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POSITRONS, QUANTUM CRYSTALS, AND NANOPARTICLES (OH MY!) – QUANTUM MECHANICS IN ACTION AT THE USAF (BRIEFING CHARTS)

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APRIL 2008

BRIEFING CHARTS

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■ **Air Force Material Command** ■ **United Air States Force** ■ **Eglin Air Force Base**

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Positrons, Quantum Crystals, and Nanoparticles (Oh My!) - Quantum Mechanics in action at the USAF

C. Michael Lindsay

Energetic Materials Branch

Air Force Research Laboratory

AFRL

THE AIR FORCE RESEARCH LABORATORY

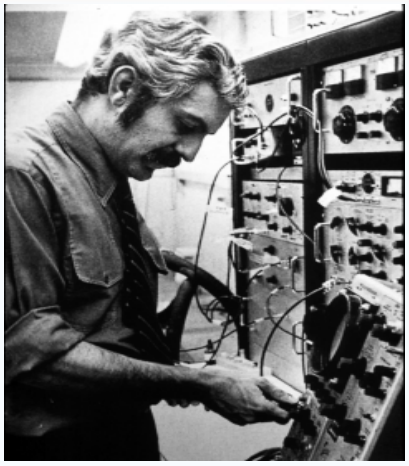
LEAD I DISCOVER I DEVELOP I DELIVER

Predicting Future Technologies

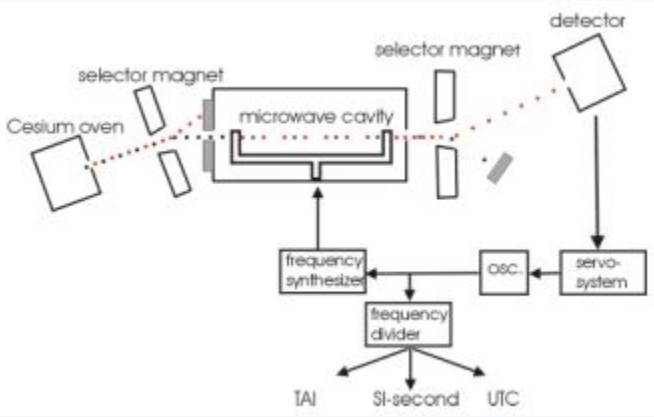
- "Nothing is less predictable than the development of an active scientific field."
  - Charles Francis Richter (1980)

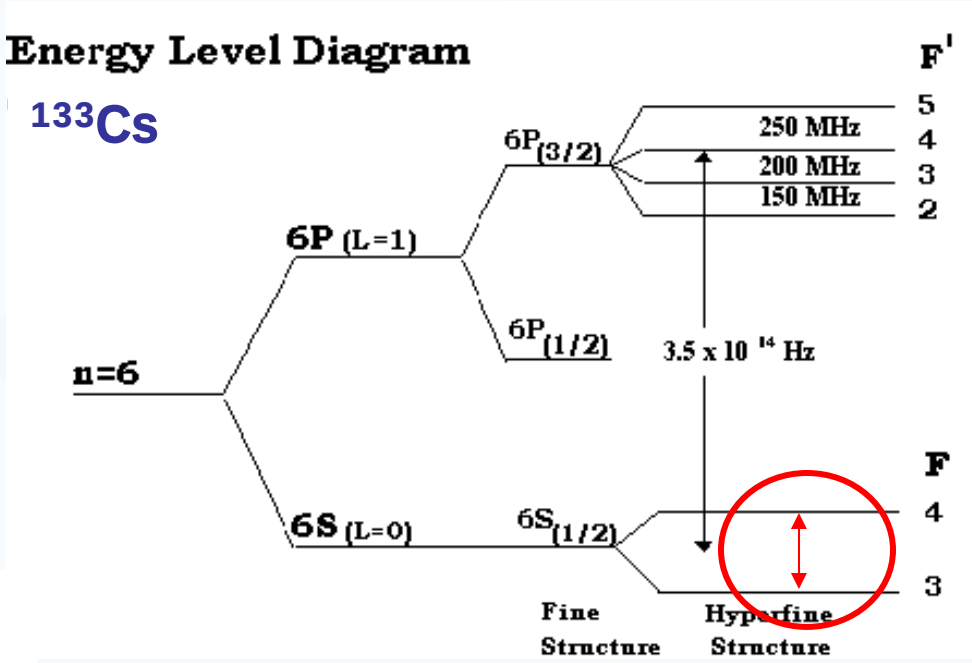
- "Trying to predict the future is like trying to drive down a country road at night with no lights while looking out the back window."
  - Peter Drucker

Case 1: Quantum Mechanics of Atoms (1937)



Isidor Isaac Rabi



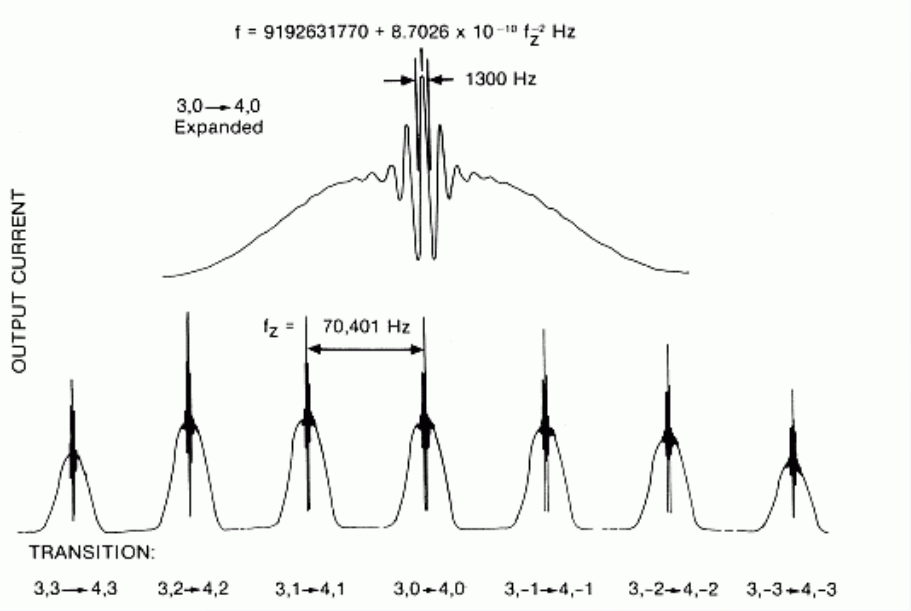


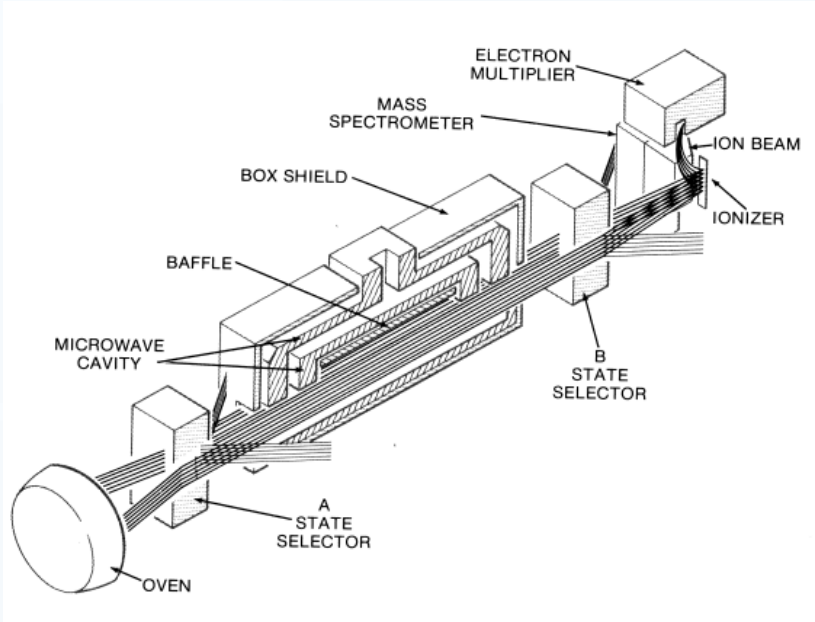
The first method for accurately measuring hyperfine frequencies by molecular beam resonance was developed by I.I. Rabi and his associates in 1937 at Columbia University

Phys. Rev. 55, 1176 - 1181 (1939)

Hyperfine structure of Cesium-133

- **9.192 631 770** GHz (Cs-133 Hyperfine Beat)

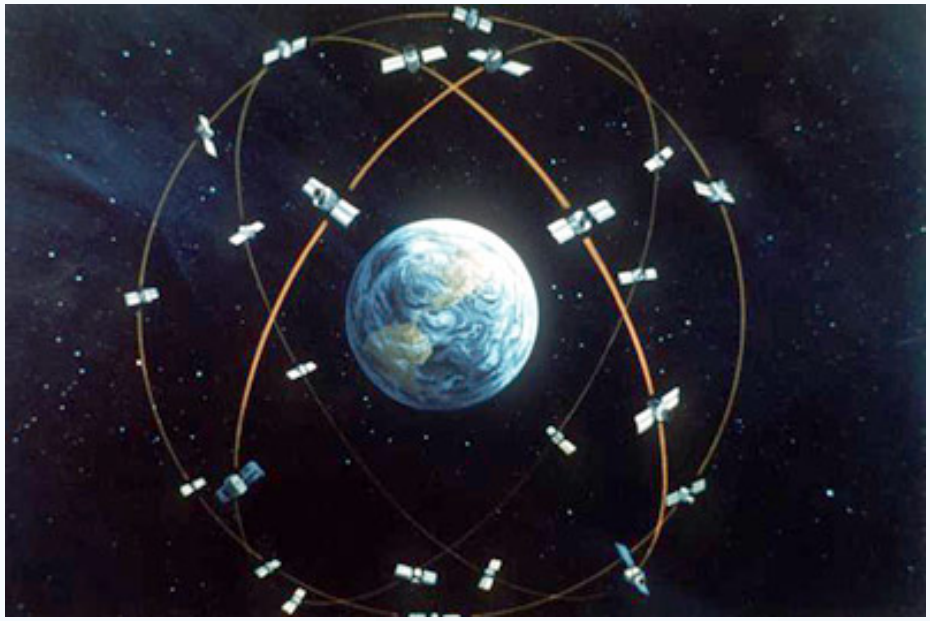




Precision of ~ 1 part in 10^{12}!

Hewlett-Packard 5062C Cesium Beam Frequency Reference Training Manual, November 1974

Enabling Technology - GPS!



- 20,000 km - 300,000 km per second
- Four satellites required to pinpoint 3-D location
- Each of the 24 GPS satellites holds four atomic clocks, which every day get an accurate time transfusion from the Air Force, which "borrows" time from the United States Naval Observatory.
- Requires 1 part in 10^{12} temporal precision in order to predict position within 1 meter

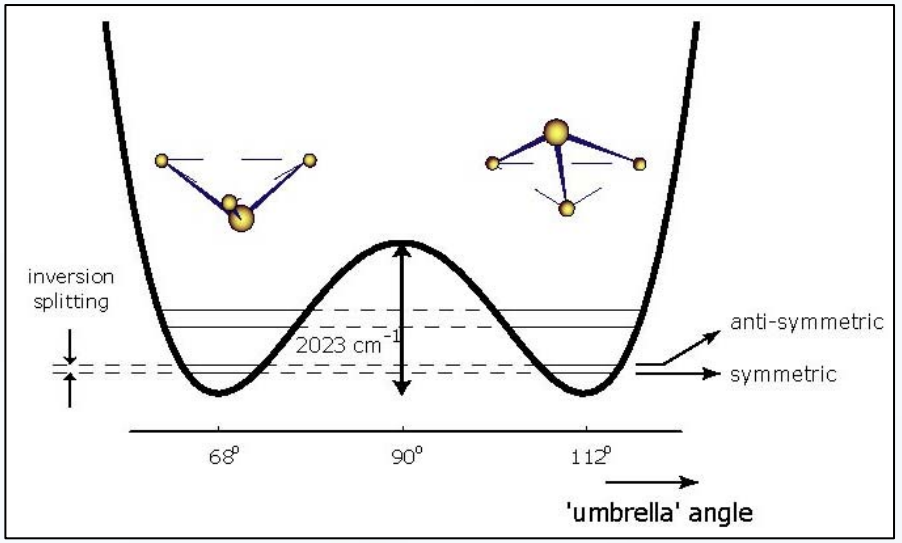
(I. I. Rabi won the Nobel Prize in Physics 1944

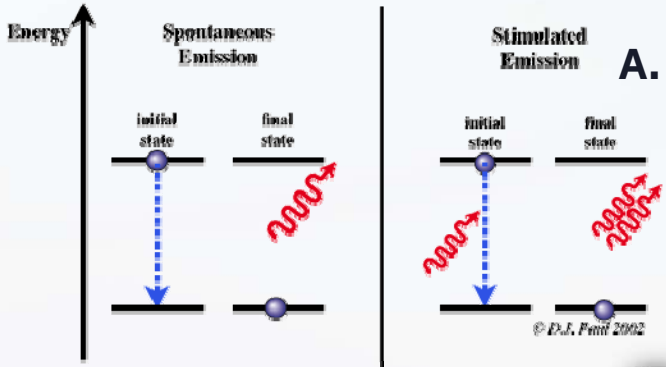
N.F. Ramsey won the Nobel Prize in Physics 1989)

AFRL

Case 2: Quantum Mechanics of Molecules (1953)

Charles Townes





A. Einstein - 1917

- Research stimulated by DoD's attempts at 1 ¼ cm RADAR

The Ammonia MASER

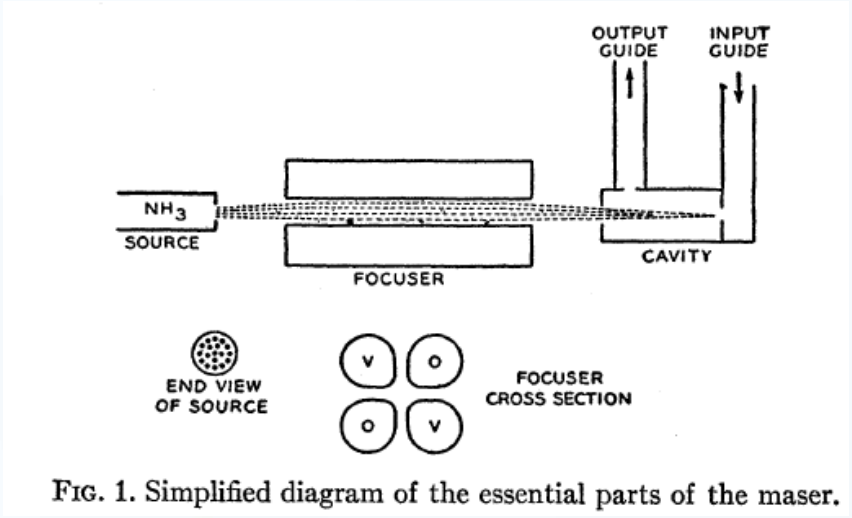


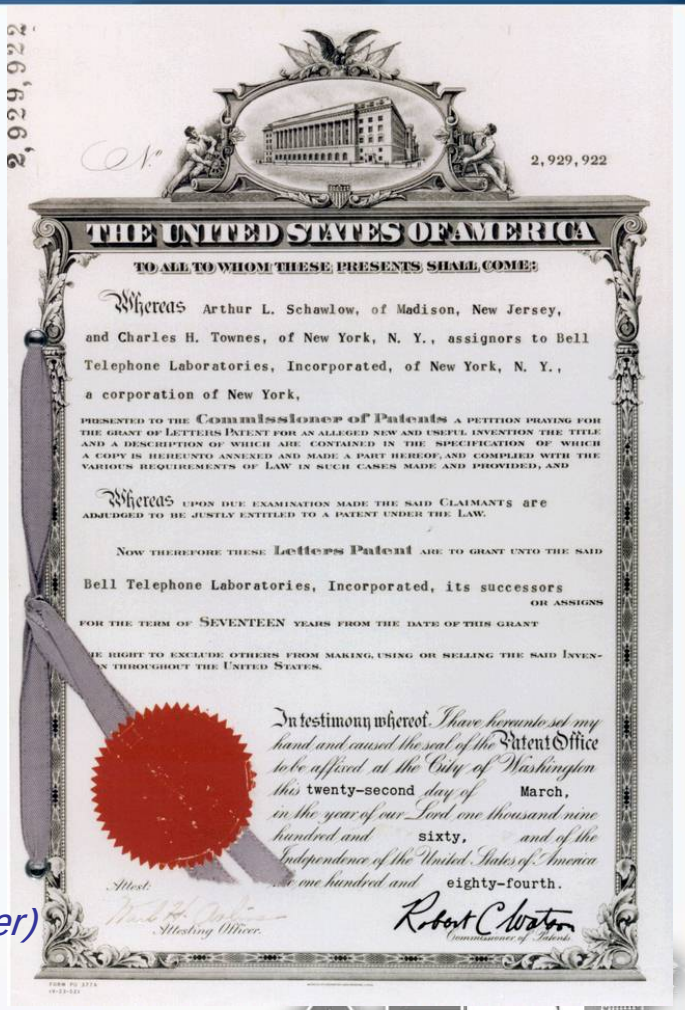
FIG. 1. Simplified diagram of the essential parts of the maser.

Description: L-R: C.H. Townes, J. P. Gordon, and T. C. Wang. Wang stands next to the first ammonia-beam maser. The second ammonia-beam maser is in front center with side removed so that internal structure can be seen. Columbia University.

Gordon, Zeiger, and Townes, Nature 318 162 (1985)

Extend MASER technique to IR and Visible

- Schawlow (Bell Labs) and Townes (consulting with Bell) realized that extending infrared or visible would be an even more powerful tool for spectroscopy.
- In 1957-58 they worked out the details on extending the MASER to the visible and applied for a patent. They were awarded a patent in 1960 and that same year Theodore Maiman (Hughes Aircraft Company) built a pulsed Ruby Laser.


2,929,922

THE UNITED STATES OF AMERICA

TO ALL TO WHOM THESE PRESENTS SHALL COME:

Whereas Arthur L. Schawlow, of Madison, New Jersey, and Charles H. Townes, of New York, N. Y., assignors to Bell Telephone Laboratories, Incorporated, of New York, N. Y., a corporation of New York,

PRESENTED TO THE Commissioner of Patents A PETITION PRAYING FOR THE GRANT OF LETTERS PATENT FOR AN ALLEGED NEW AND USEFUL INVENTION THE TITLE AND A DESCRIPTION OF WHICH ARE CONTAINED IN THE SPECIFICATION OF WHICH A COPY IS HEREUNTO ANNEXED AND MADE A PART HEREOF, AND COMPLIED WITH THE VARIOUS REQUIREMENTS OF LAW IN SUCH CASES MADE AND PROVIDED, AND

Whereas UPON DUE EXAMINATION MADE THE SAID CLAIMANTS are ADJUDGED TO BE JUSTLY ENTITLED TO A PATENT UNDER THE LAW.

NOW THEREFORE THESE Letters Patent ARE TO GRANT UNTO THE SAID Bell Telephone Laboratories, Incorporated, its successors OR ASSIGNS FOR THE TERM OF SEVENTEEN YEARS FROM THE DATE OF THIS GRANT THE RIGHT TO EXCLUDE OTHERS FROM MAKING, USING OR SELLING THE SAID INVENTION THROUGHOUT THE UNITED STATES.

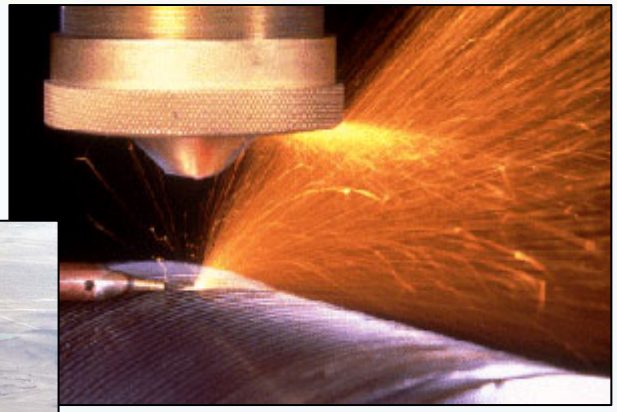
In testimony whereof I have hereunto set my hand and caused the seal of the Patent Office to be affixed at the City of Washington this twenty-second day of March, in the year of our Lord one thousand nine hundred and sixty, and of the Independence of the United States of America the one hundred and eighty-fourth.

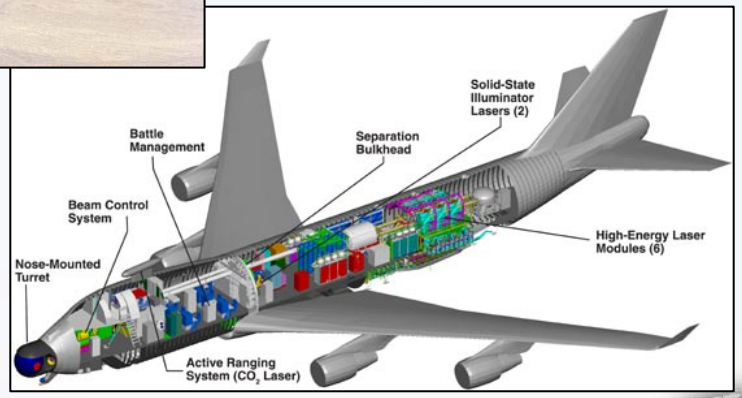
Attest: Attesting Officer. Robert C. Watson Commissioner of Patents

Charlie Townes – Nobel Prize in Physics – 1964 (Maser/laser amplifier)
Arthur Schawlow – Nobel Prize in Physics – 1981 (develop. of laser)

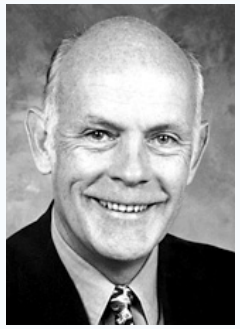
Military Applications of Lasers

- Laser guided munitions
- Laser machining
- Laser sights
- Airborne laser
- Laser ranging
- …

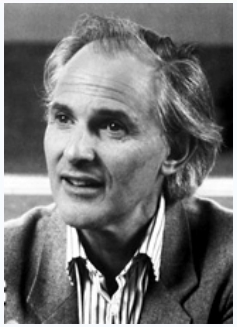




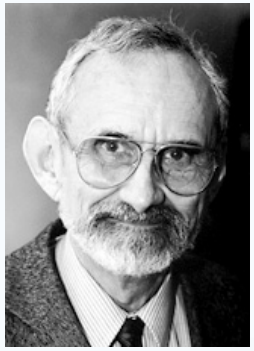
Case 3: Unidentified Spectra in Interstellar Clouds



Richard Smalley



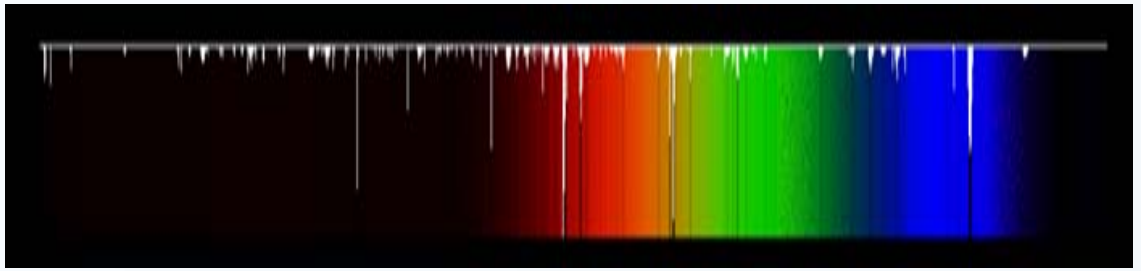
Harry Kroto



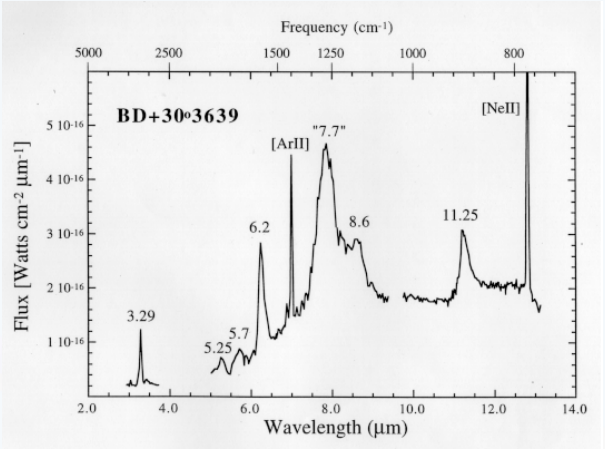
Robert Curl

Proposed that carbon clusters were a source of interstellar spectral features

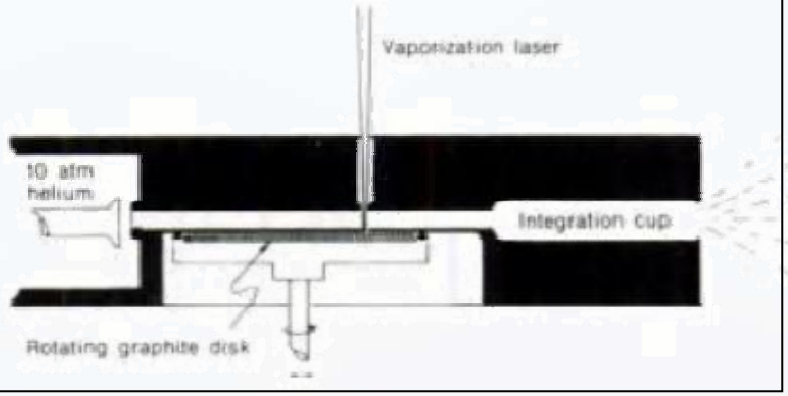
Diffuse Interstellar Bands



Unidentified Infrared Bands



Carbon Cluster Apparatus



C_{60}: Buckminsterfullerene

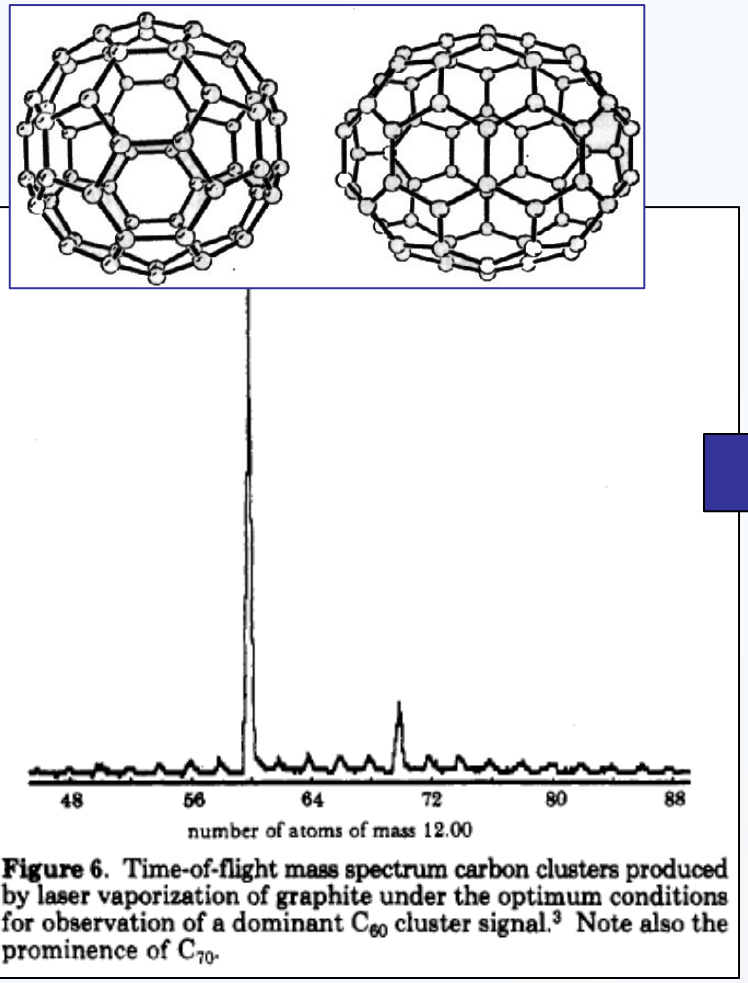
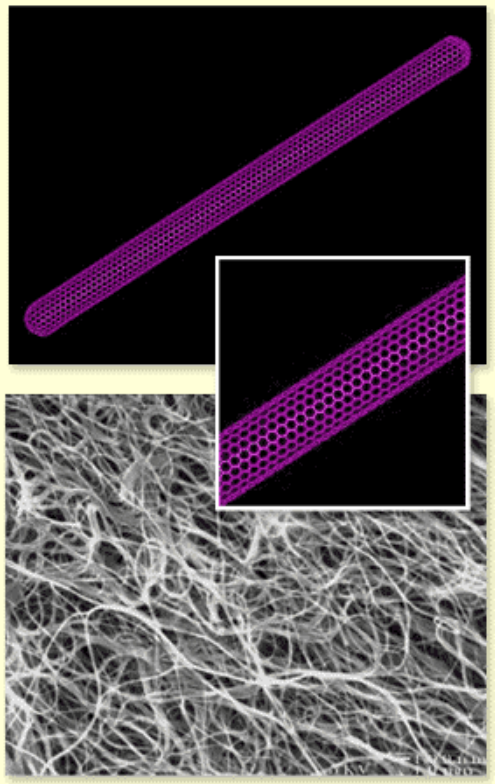


Figure 6. Time-of-flight mass spectrum carbon clusters produced by laser vaporization of graphite under the optimum conditions for observation of a dominant C_{60} cluster signal.[3] Note also the prominence of C_{70}.

MOLECULAR PERFECTION:

THE FULLERENE IDEAL

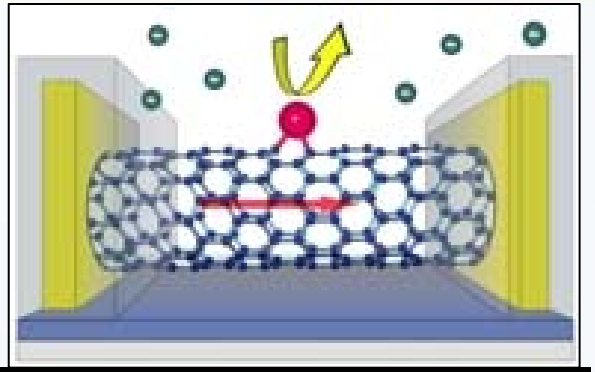
1. The strongest fiber that will be ever made
2. Electrical Conducivity of Copper or Silicon
3. Thermal Conducivity of Diamond
4. The Chemistry of Carbon
5. The size and perfection of DNA

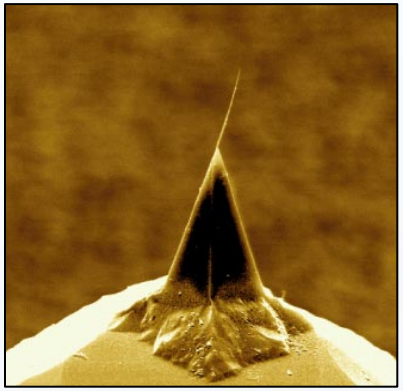


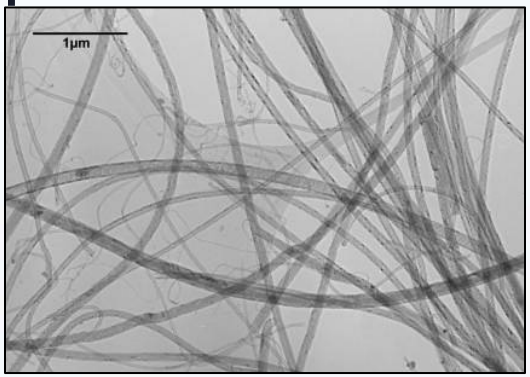
Kroto, *et al.* Nature 318 162-163 (1985)

(Near-Future) Applications of Carbon Nanotubes

- Fuel storage (H_2, CH_4, etc...)
- Structural composite materials
- Ultra-high conductivity electronics
- Ultra efficient field induced electron emitters
- Conductive plastics







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More Serendipitous Discoveries…

Chemistry

- **Polyethylene** by Hans von Pechmann, who prepared it by accident in 1898 while heating diazomethane
- **Teflon,** by Roy J. Plunkett, who was trying to develop a new gas for refrigeration and got a slick substance instead, which was used first for lubrication of machine parts
- **Cyanoacrilate** glue(a.k.a. Superglue) was accidentally twice discovered by Dr. Harry Coover, first when he was developing a clear plastic for gunsights and later, when he was trying to develop a heat-resistant polymer for jet canopies.
- **Aspartame** (a.k.a. NutraSweet) was also accidentally ingested by G.D. Searle chemist James Schlatter, who was trying to develop a test for an anti-ulcer drug.

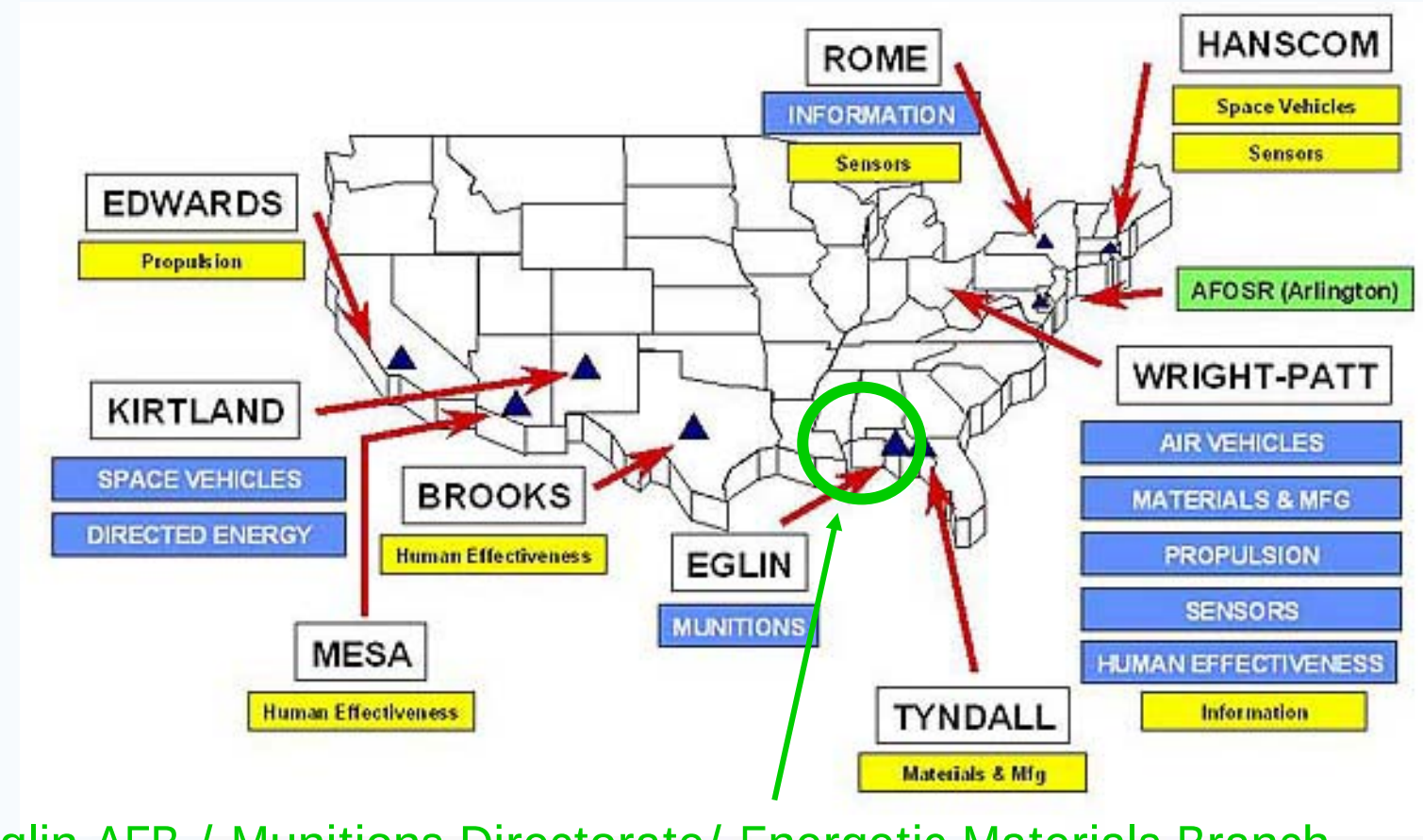
Physics

- **Radioactivity**, by Henri Becquerel. While trying to investigate phosphorescent materials using photographic plates, he stumbled upon uranium.
- **X rays**, by Wilhelm Roentgen. Interested in investigating cathodic ray tubes, he noted that some fluorescent papers in his lab were illuminated at a distance
- **Electromagnetism**, by Hans Christian Oersted. While he was setting up his materials for a lecture, he noticed a compass needle deflecting from magnetic north when the electric current from the battery he was using was switched on and off.
- The **thermoelectric effect** was discovered accidentally by Estonian physicist Thomas Seebeck, in 1821, who found that a voltage developed between the two ends of a metal bar when it was submitted to a difference of temperature.

Technology

- Discovery of the principle behind **inkjet printers** by a Canon engineer. After putting his hot soldering iron by accident on his pen, ink was ejected from the pen's point a few moments later.
- The **microwave oven** was invented by Percy Spencer while testing a magnetron for radar sets at Raytheon, he noticed that a peanut candy bar in his pocket had melted when exposed to radar waves.
- **Post-it Notes** by Spencer Silver and Arthur Fry. They tried to develop a new glue at 3M, but it would not dry. So they devised a new use for it.

Air Force Research Laboratory



- Eglin AFB / Munitions Directorate/ Energetic Materials Branch

AFRL/RWMER – LASEM Lab

Laboratory for **A**pplied **S**pectroscopy of **E**nergetic **M**aterials

New Basic and Applied Research Team at Eglin AFB (~ 4 years old)

Team Members (but expanding)

- **PI's (Physical Chemists)**
- **NRC Post docs**
  (Materials and Physical chemists)
- **Millitary Officers (A-Chemist, P-Chemist and a Physicist)**
- **Technicians**
- **(3-4 Open Postdoc Positions)**

AFRL/RWMER – LASEM Lab

Laboratory for **A**pplied **S**pectroscopy of **E**nergetic **M**aterials

Research Areas

- Explosives
- Reactive composite materials
- Thermite and inter-metallic materials
- Energetic thin films
- Cryogenic matrices
- Energetic core-shell nanoparticles
- Positron/plasma/positronium storage

Diagnostics

- Vis, FIR, MIR, NIR spectroscopy
- γ-ray spectroscopy
- Positron spectroscopy
- Matrix isolation spectroscopy
- TOF/QMS – mass spectrometry
- XRF/XRD
- SEM, optical microscopy
- Radiographic imaging

Cryogenic Matrices – Basic Research Interests

- Ultra-low temperature chemistry – synthesize systems under different conditions than ambient
- Energy dissipation – stabilize pre-reactive systems
- Quantum Condensed Phases – unusual properties
  - Powerful annealing behavior
  - Unprecidentedly sharp transitions
  - Superfluidity

    liquid helium, solid parahydrogen
- New regime for exploration – many surprises

Introduction - Antimatter Giggle Factor

One vision of bulk antimatter storage in the 23rd century.

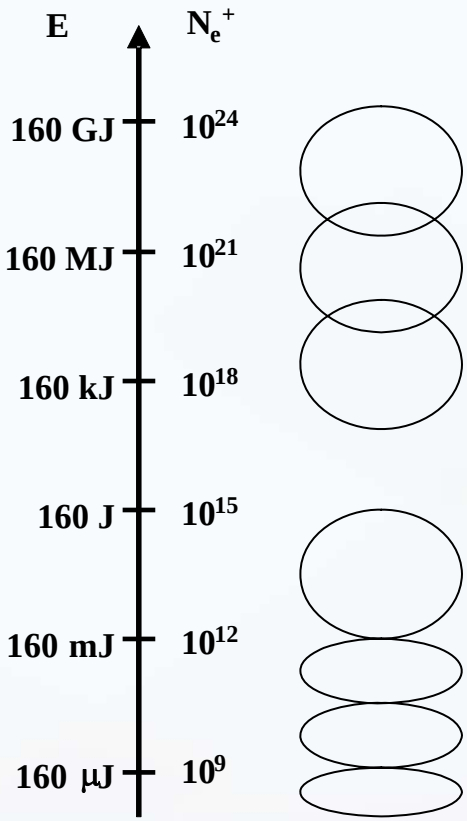
Star Trek Episode # 47 “Obsession” (Paramount, 1967).

Skepticism of near-term practical energy storage is justified.

Introduction - Reality Check

Annihilation energy:
$E = 2\, N_{e+}\, m_e c^2$

Brillouin (B ~ 1 T) and Space Charge (V ~ 100 kV) → limits on bare e^+ storage in ~ 1 m^3



	far-term (breakthrough physics required)
tabletop γ-laser	mid-term (10-15 years)
Ps BEC demo	near-term
Ps_2 formation demo	Mills, UCR !
state of the art	Surko, UCSD

e^+ = positron; Ps = positronium (e^+/e^- bound pair);
PEC = Positron Energy Conversion Project; BEC = Bose-Einstein Condensation

Introduction - Positron Moderation

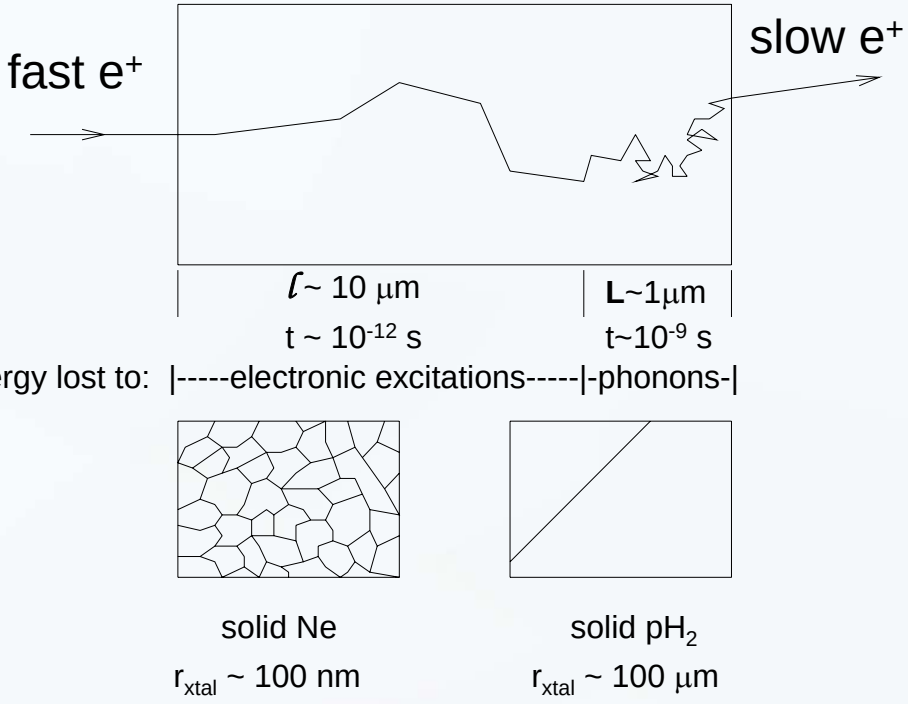
Generic positron production scheme:
- (1) nascent fast e^+ (E ~ 100 keV)
- (2) moderation (E ~ 1 eV)
- (3) e^+ and/or Ps trapping

Solid Ne is best known moderator
$\varepsilon \approx 0.5$ %; so 99.5 % are wasted

Slow e^+ scatter, trap, and annihilate at defects $\Rightarrow$ lost to moderation process

High quality parahydrogen (pH_2) solids should permit slow positrons to emerge from deeper within moderator

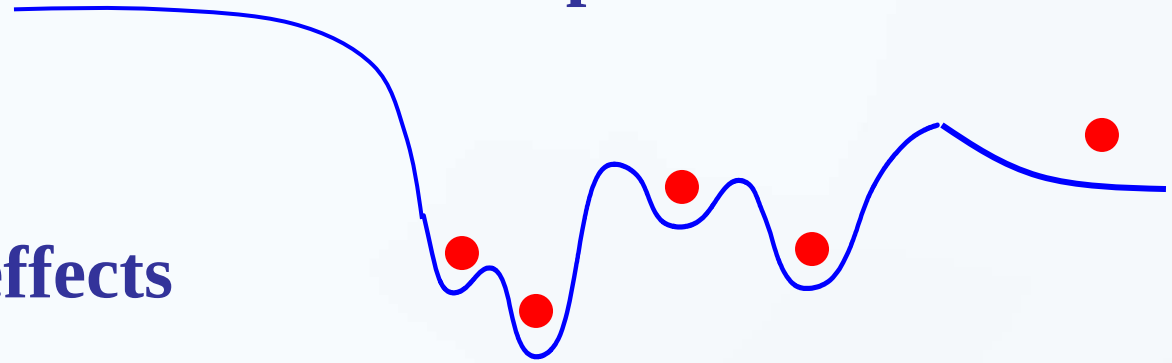
Moderation efficiency increases as L / ℓ



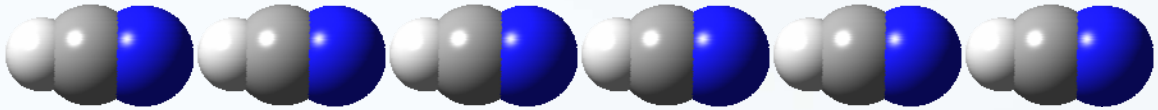
[E.M. Gullikson and A.P. Mills, Jr., Phys. Rev. Lett. **57**, 376 (1986)]

Ultra-low Temperature Chemistry

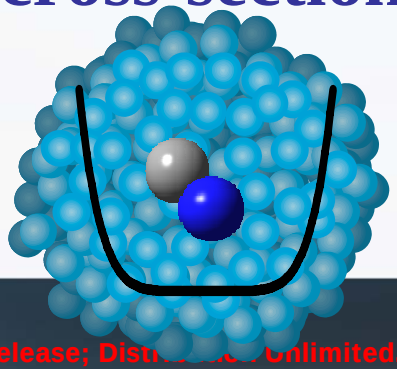
- Reactions occur in a dissipative environment



- Steric effects



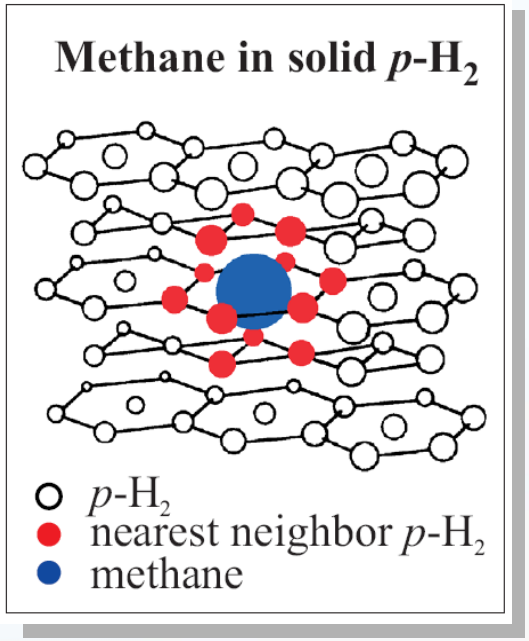
- Large “reaction” cross-sections



About solid parahydrogen

Solid parahydrogen features:

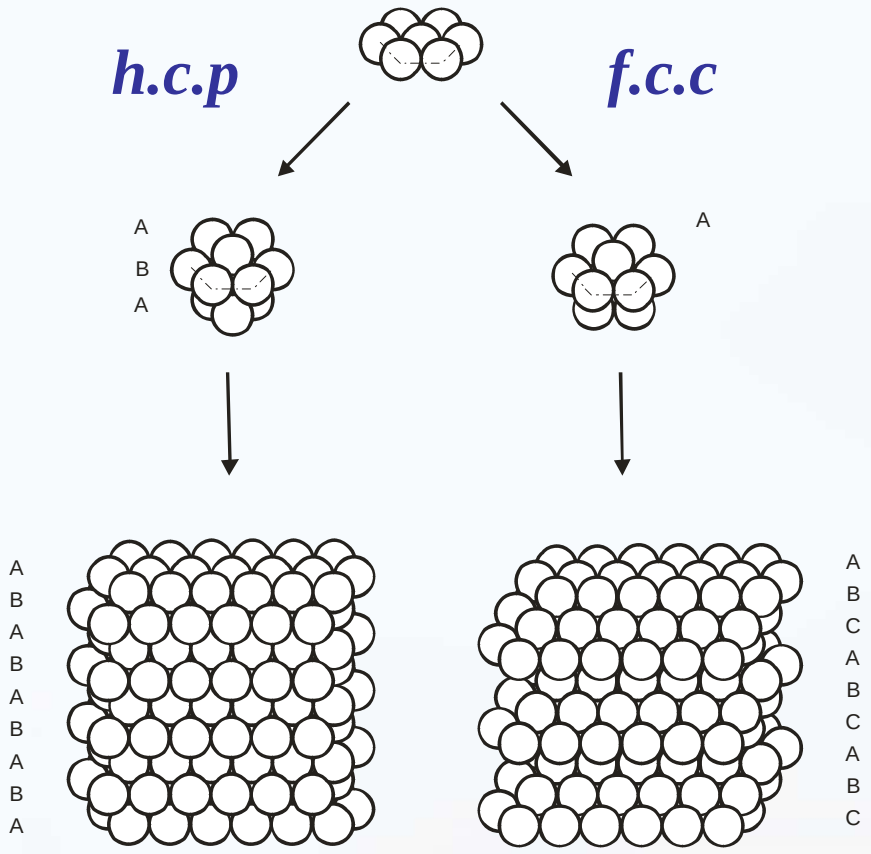
- Weak intermolecular interactions
- Slow relaxation timescales
- Quantum crystal: self-annealing via tunneling
- Homogeneous environment
- Large intermolecular distance, 3.78 Å



Parahydrogen as a matrix:

- Very small matrix shifts, predictable (-0.5 %)
- Nearly free rotation for small molecules
- High impurity mobility
- Narrow spectral linewidths (<100 MHz possible)
- Dopants induce infrared activity in matrix

Close packing crystal structure

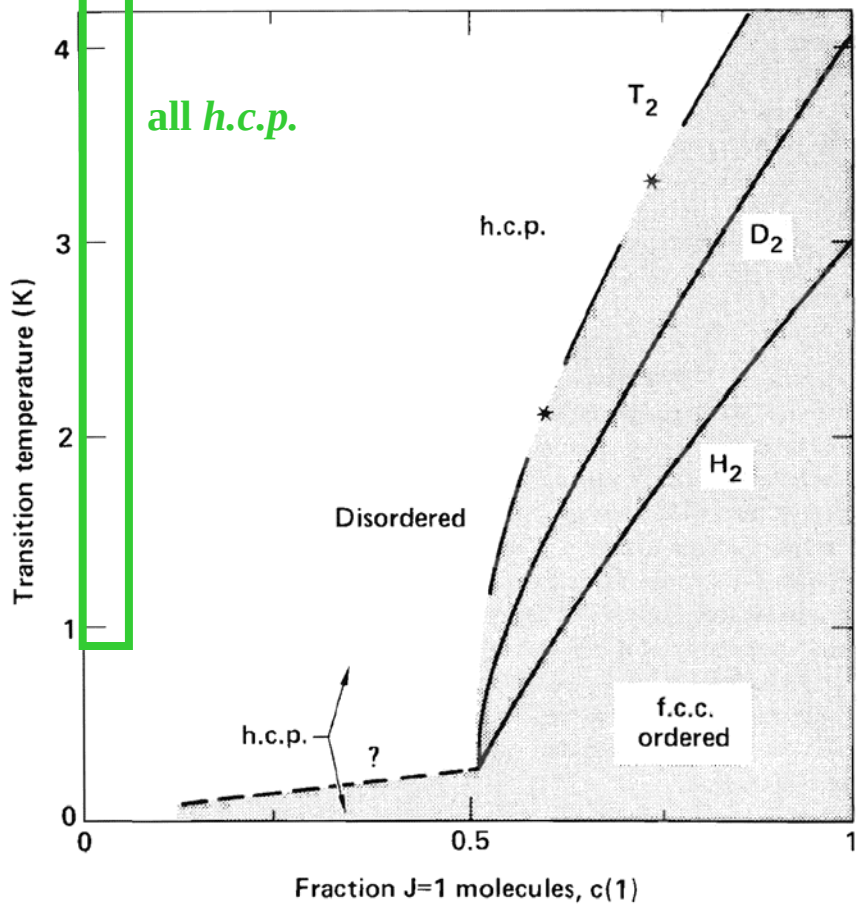


- **Symmetry:** $h.c.p. - D_{3h}$; $f.c.c. - O_h$
- **Reduced symmetry in *h.c.p.* provides directionality to the crystal and thus enables polarization sensitive measurements to be performed.**
- **Relative stability of *f.c.c.* and *h.c.p.* structures depends on many-body long-range interactions.**
- **Most stable structure in rare gas solids (RGS) is *f.c.c.* ***

*** Excluding solid helium**

Adapted from P. C. Souers, *Hydrogen Properties for Fusion Energy*, (1986)

f.c.c versus *h.c.p.*

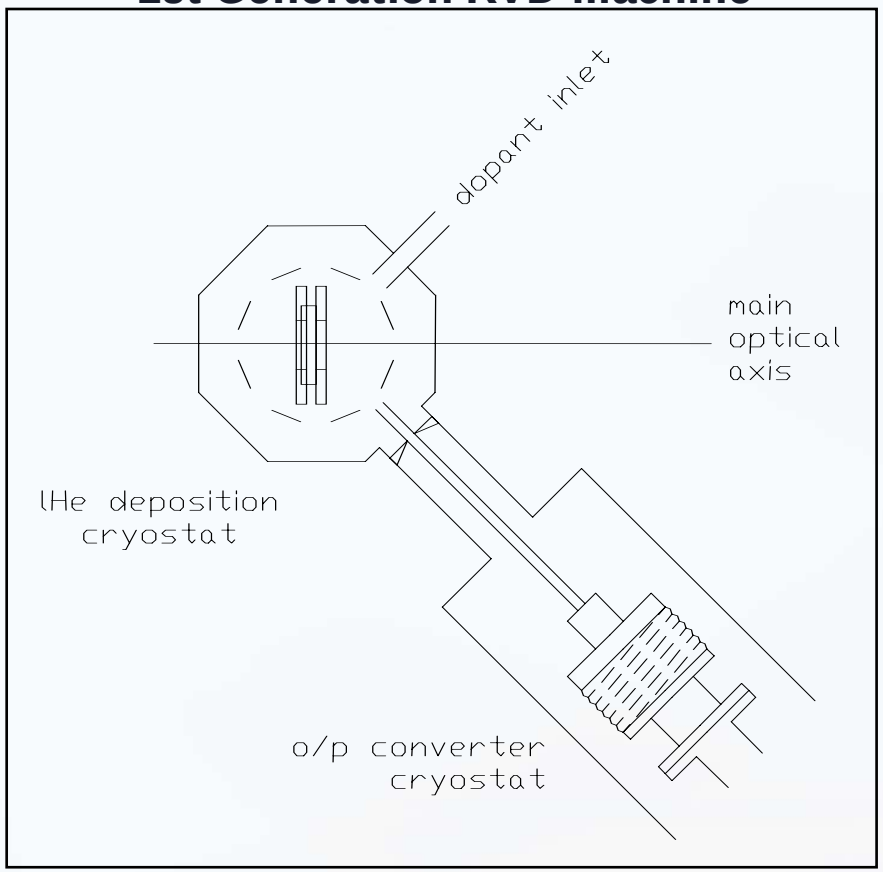


- Unlike RGS, solid parahydrogen (J=0) has *h.c.p.* as the lowest energy crystal structure.
- *h.c.p* more stable than *f.c.c.* by ~1 mK per molecule.
- Solid parahydrogen synthesized by rapid vapor deposition at low temperature produces a mixture of *f.c.c.* and *h.c.p.* phases. Nearly exclusive *h.c.p.* structure produced upon annealing above ~ 4.5 K.

P. C. Souers, *Hydrogen Properties for Fusion Energy*, (1986).
J. Van Kranendonk, *Solid Hydrogen*, (1983).

Rapid Vapor Deposition

1st Generation RVD machine



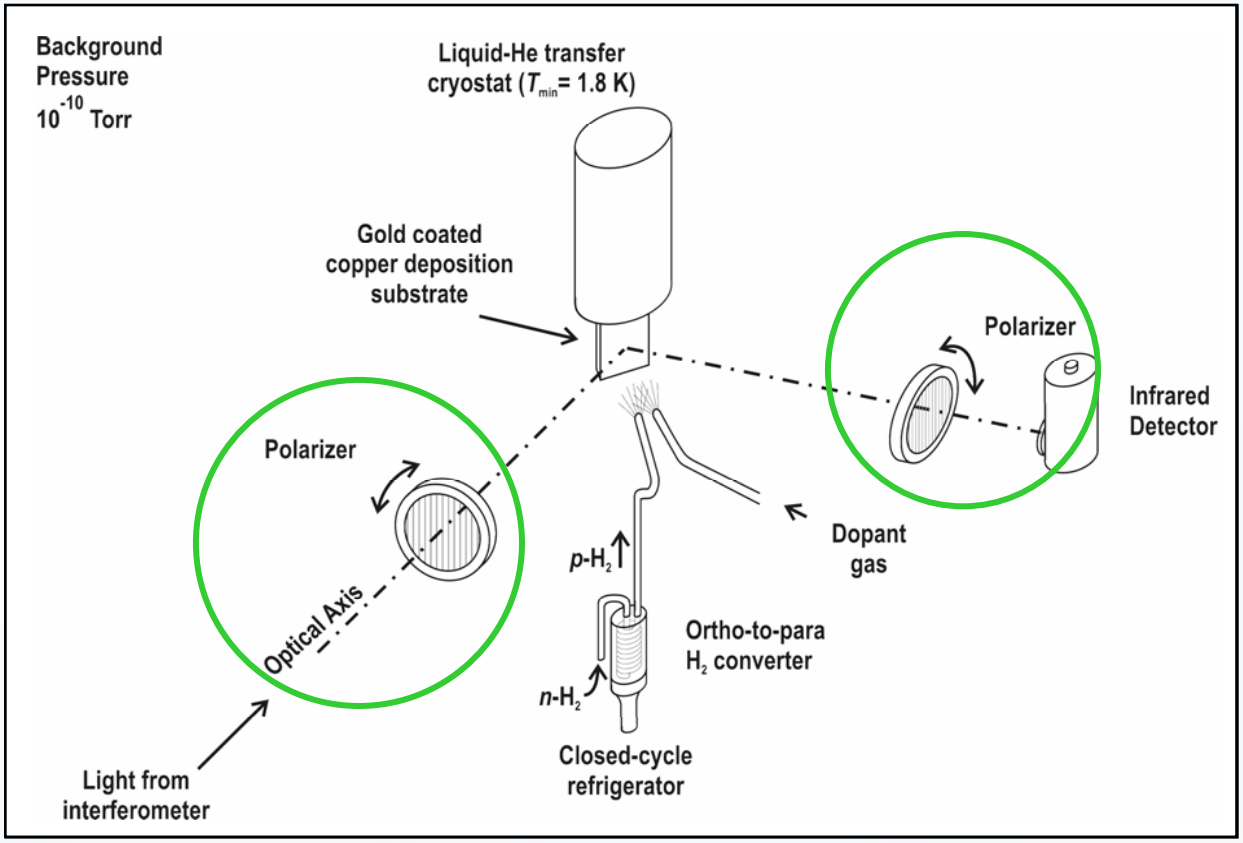
- Original machine built at Edwards AFB in 1995.
- Optical path normal to substrate.
- Rotating molecules: $\Delta m = 0$ transitions suppressed relative to $\Delta m = \pm 1$

M.E. Fajardo and S. Tam, *J. Chem. Phys.* **108**, 4237 (1998).
S. Tam and M.E. Fajardo, *Rev. Sci. Instrum.* **70**, 1926 (1999).

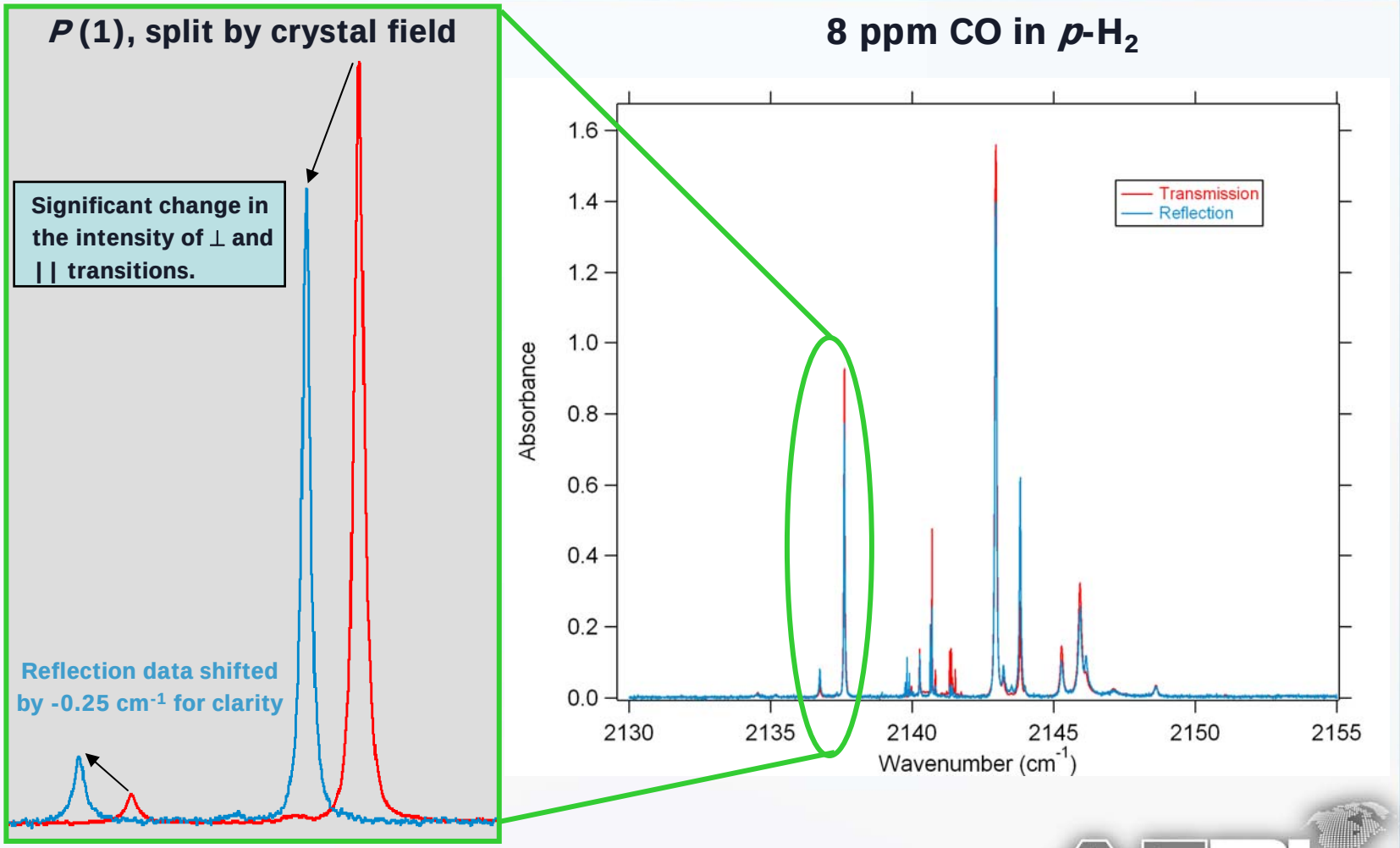
Eglin AFB Rapid Vapor Deposition Instrument

- Reflection based set-up (FTIR).
- [*o*-H_2] < 100 ppm.
- *p*-H_2 deposition rate ~150 mmol/hr → 2-3 mm/hr thickness.
- Deposition at 2.3 K. Sample annealed at 4.3 K for 15-30 min.

2nd Generation RVD machine

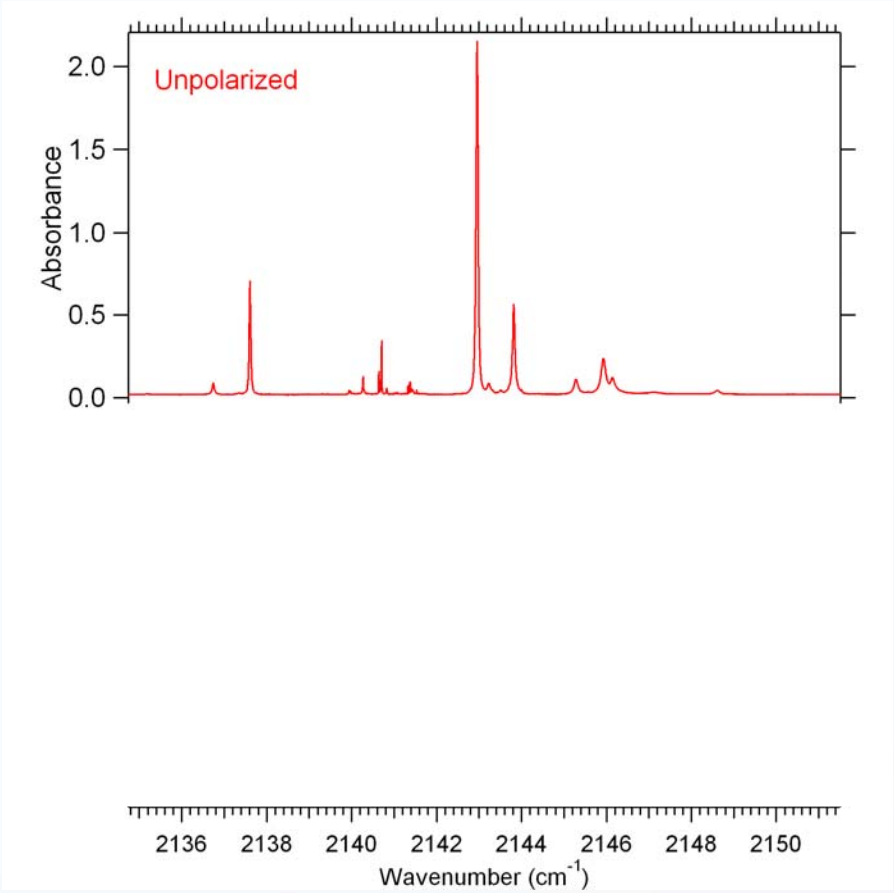


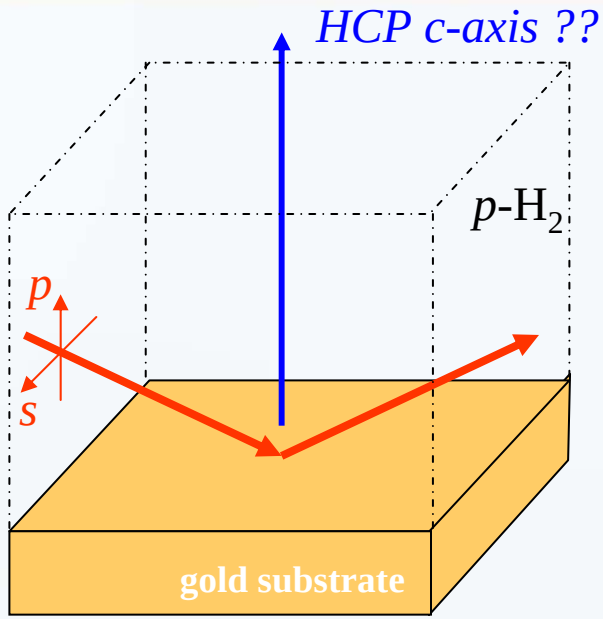
Optical Geometry: Reflection Versus Transmission



Polarization Spectroscopy

8 ppm CO in *p*-H2

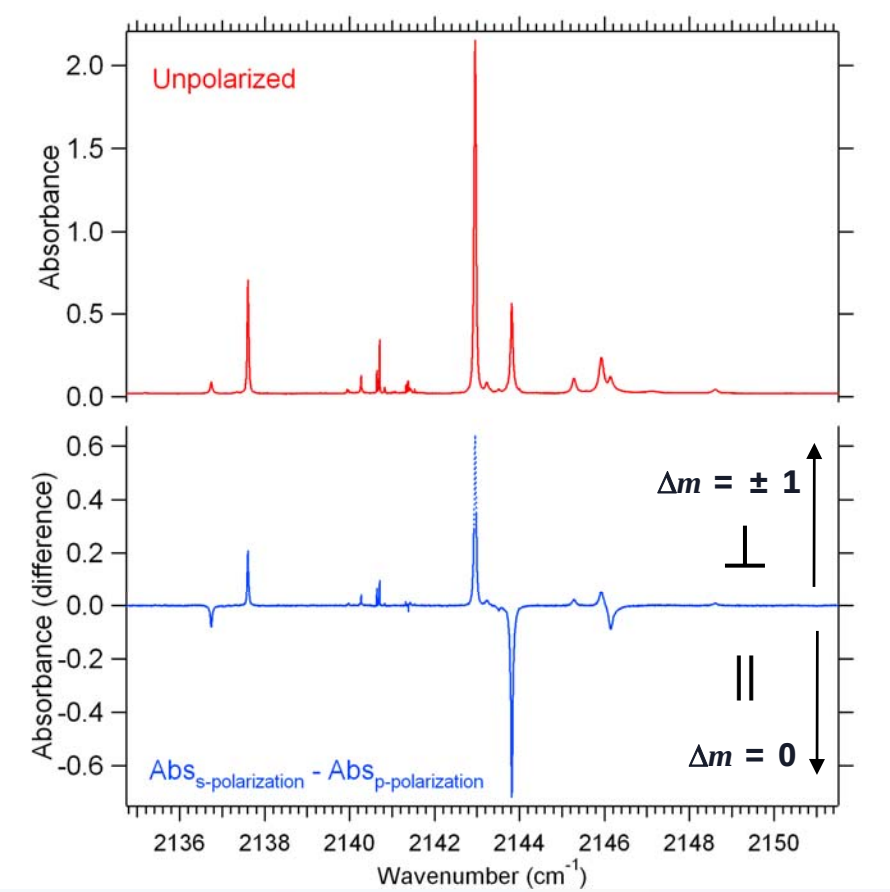


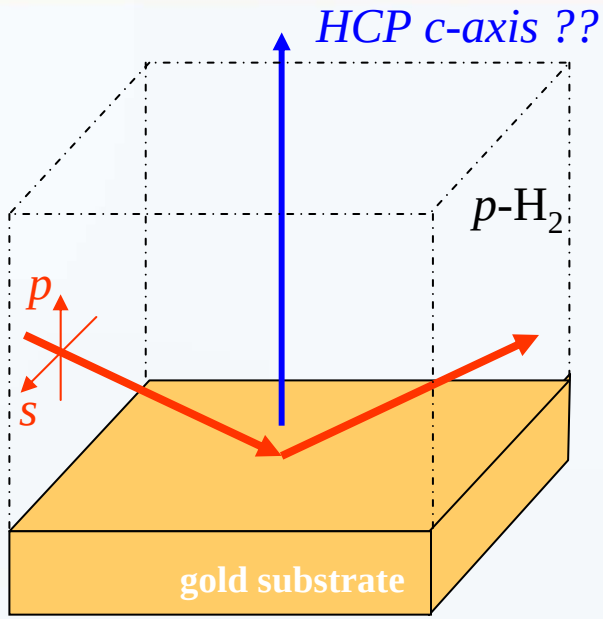


Polarization analysis provides:

- **An assignment of the perpendicular and parallel components to the crystal field perturbed rotational structure (*i.e.* Δm)**
- **$Abs_{s\text{-}pol} - Abs_{p\text{-}pol} = \frac{1}{2}\mu^2_{\perp} - \frac{1}{2}\mu^2_{\parallel}$**

Polarization Spectroscopy





Polarization analysis provides:

- **An assignment of the perpendicular and parallel components to the crystal field perturbed rotational structure (*i.e.* Δm)**
- **$Abs_{s\text{-}pol} - Abs_{p\text{-}pol} = \frac{1}{2}\mu^2_{\perp} - \frac{1}{2}\mu^2_{\parallel}$**

Rotation of “Large” Molecules in Solid Parahydrogen

Rotation in the Solid Matrices

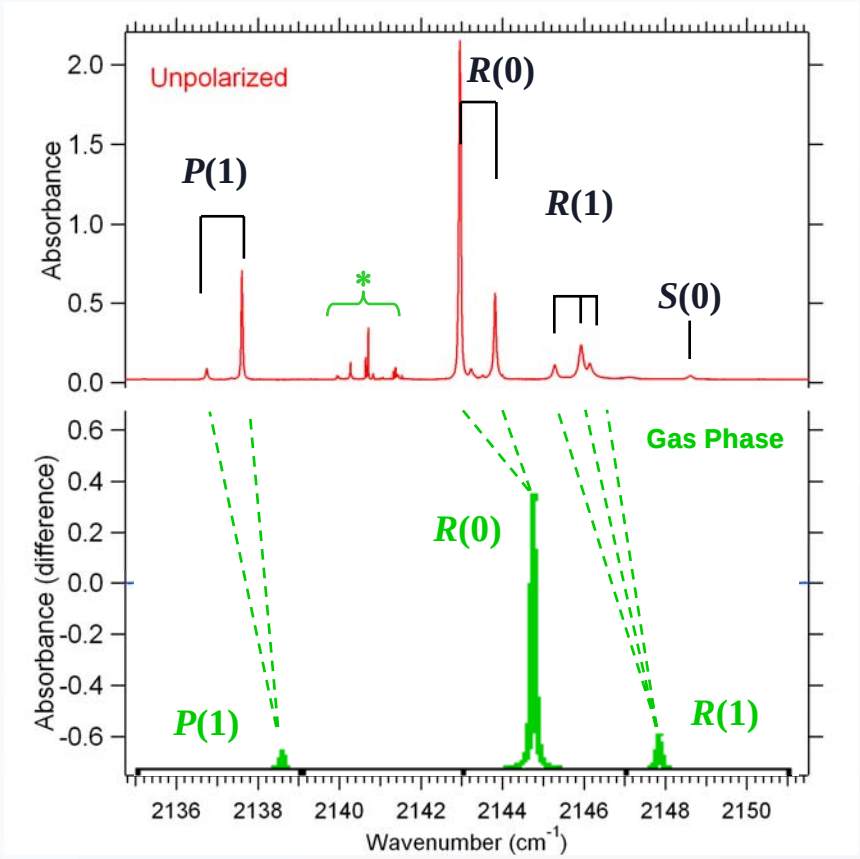
- Rare gas matrices and traditional molecular matrices:
  - Small hydrides: HX, H_2O, NH_2, NH_3, CH_3, CH_4
  - *Perhaps* ClF, CN (ESR and IR spectra conflict)

- Solid parahydrogen:
  - Very low angular anisotropy, and weak intermolecular interactions
  - Small hydrides: HX, H_2O, NH_3, CH_3, CH_4
  - "*Large*" molecules: N_2, O_2, CO, NO, HCN, … *more*?

Narrow spectral lines widths and the ability to examine the rotation of larger molecules allows us to examine the impurity-matrix interactions with remarkable clarity

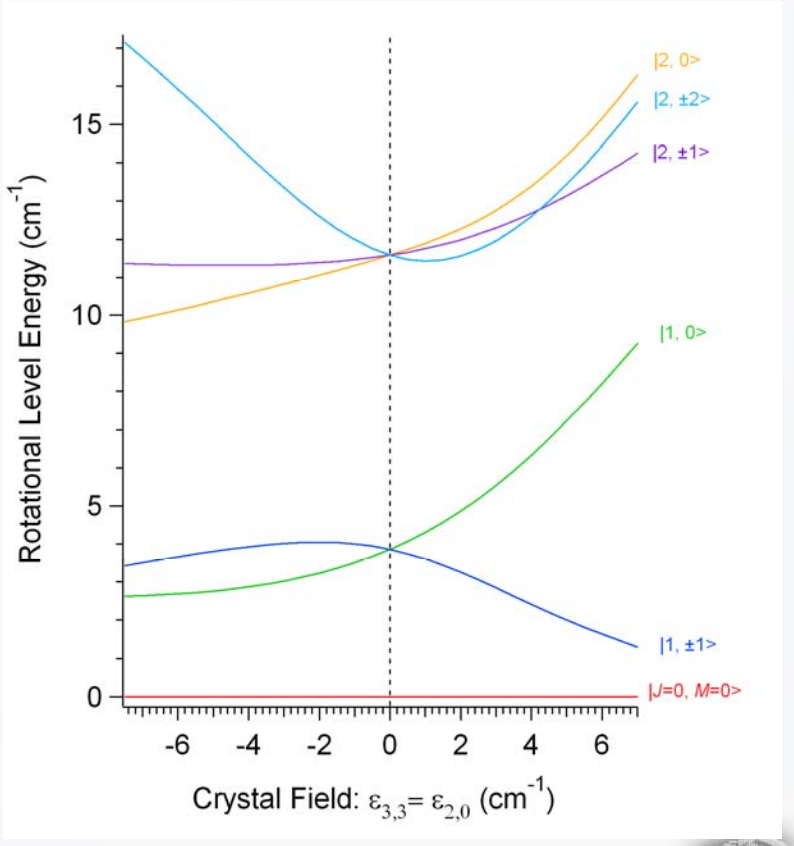
CO and HCN in parahydrogen

8 ppm CO in *p*-H_2



Simulation:

Linear molecule in *h.c.p* crystal field

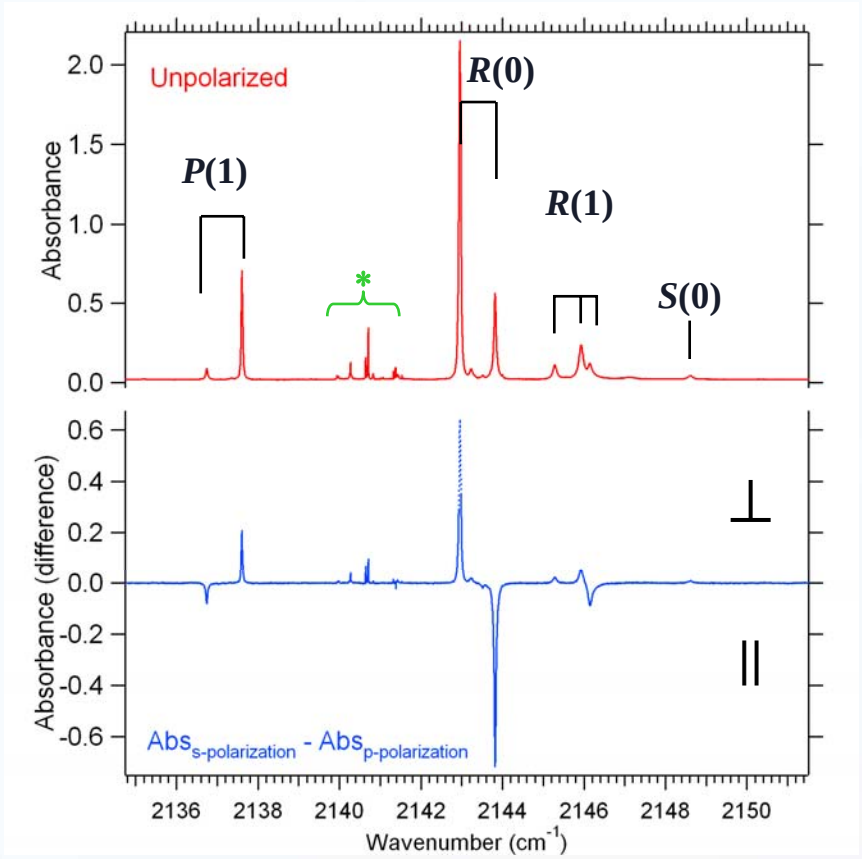


* *o*-H_2 clustering

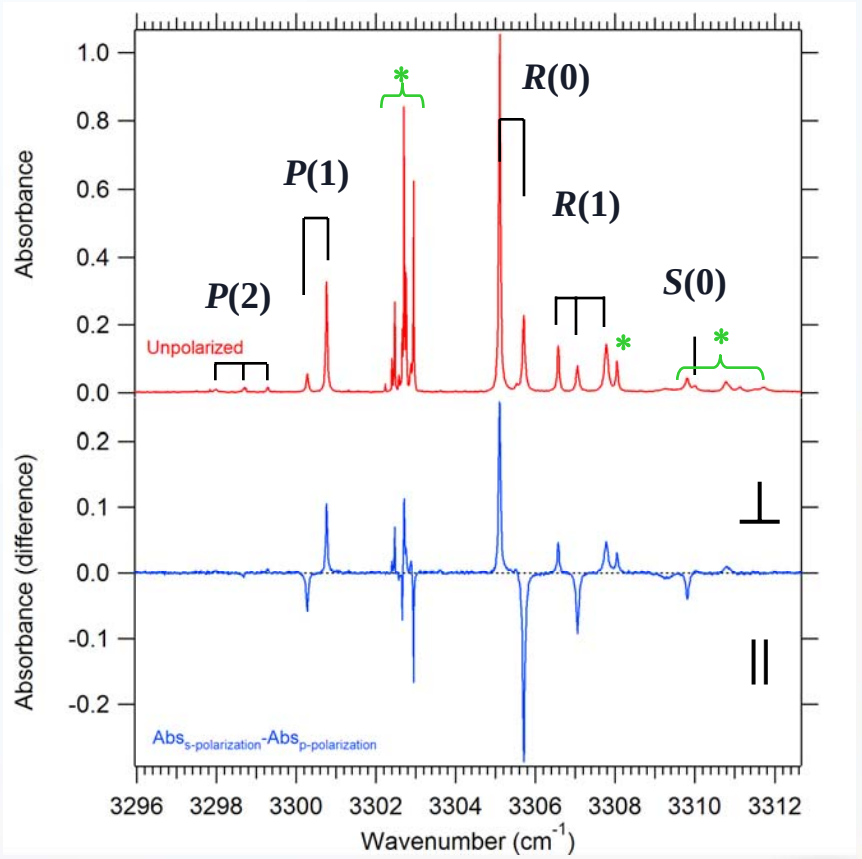
Simulation uses theory of: Devonshire, Proc. Roy. Soc. London A 153, 601 (1936); Bowers and Flygare, J. Chem. Phys., 44, 1389 (1966).

CO and HCN in parahydrogen

8 ppm CO in *p*-H_2

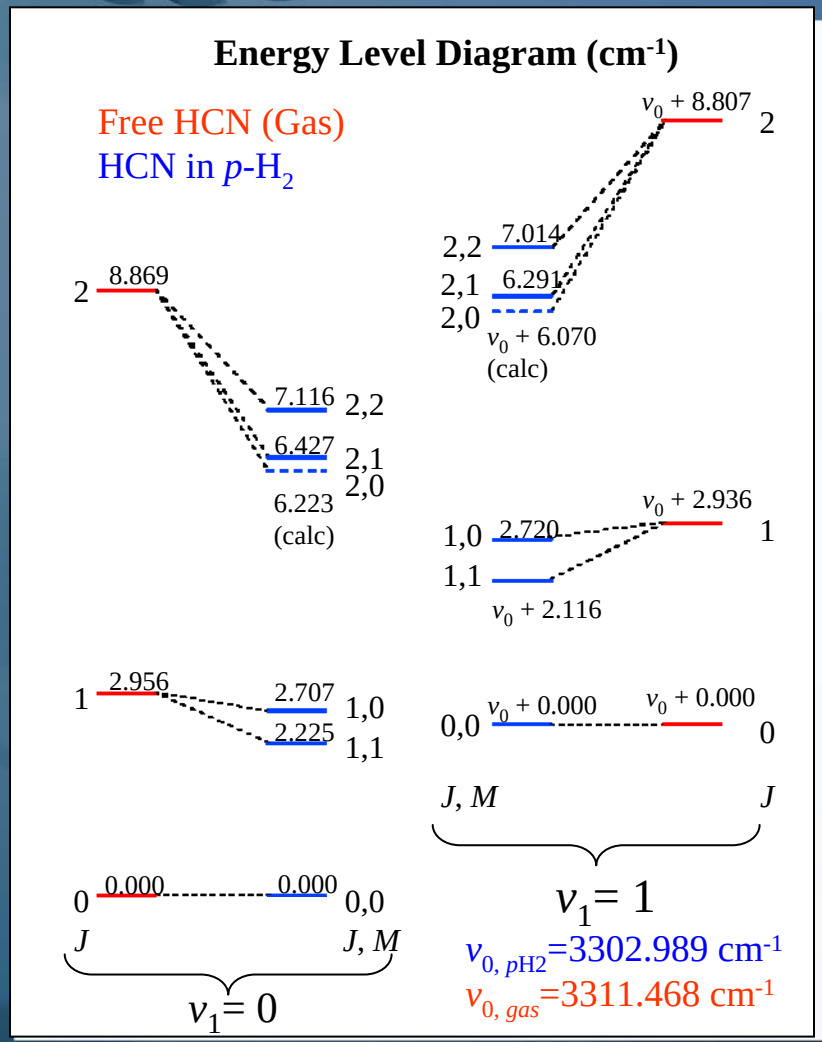


8 ppm HCN in *p*-H_2



* *o*-H_2 clustering

Interpretation of the Rotational Fine Structure- HCN



Crystal field theory (linear molecule in HCP lattice) *

$$H = H_{r,v} + V_{cry}$$

$$V_{cry} = \varepsilon_2 C_{2,0}(\Omega_{HCN}) + \varepsilon_3 [C_{3,-3}(\Omega_{HCN}) - C_{3,3}(\Omega_{HCN})]$$

$$\text{where } C_{l,m}(\Omega) = \left(\frac{4\pi}{2l+1}\right)^{1/2} Y_{l,m}(\Omega)$$

"Fitting" Results in cm^{-1}: (10 levels, 9 parameters)

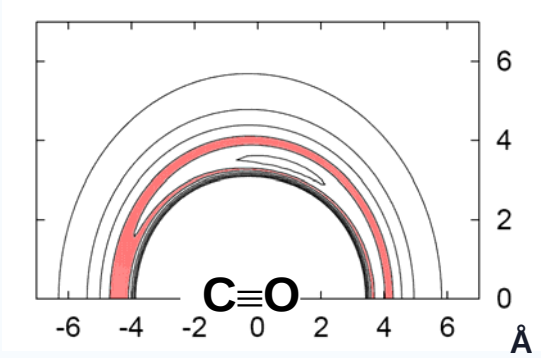
	p -H_2	Gas	
B	1.475(5)	1.478	Identical!
ΔB	-0.005(5)	-0.010	
D	0.0675(5)	2.910×10^{-6}	× 20,000!
ΔD	0.0032(5)	0.025×10^{-6}	
ν_0	3302.989(5)	3311.4770	
ε_2	-1.274(5)	-	very large!
$\Delta\varepsilon_2$	-0.193(5)	-	
ε_3	6.850(5)	-	
$\Delta\varepsilon_3$	0.767(5)	-	

NOTE: Above perturbation does not converge for large *D*! Treatment was modified to incorporate centrifugal distortion after crystal field calculation to avoid this problem.

Devonshire, Proc. Roy. Soc. London A 153, 601 (1936); Bowers and Flygare, J. Chem. Phys., 44, 1389 (1966).

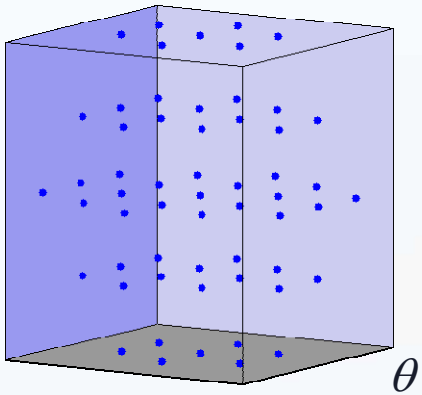
Prediction of Crystal Field Parameters: Truncation

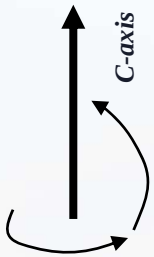
H_2-CO pair potential *



+

H_2 – *h.c.p.* lattice

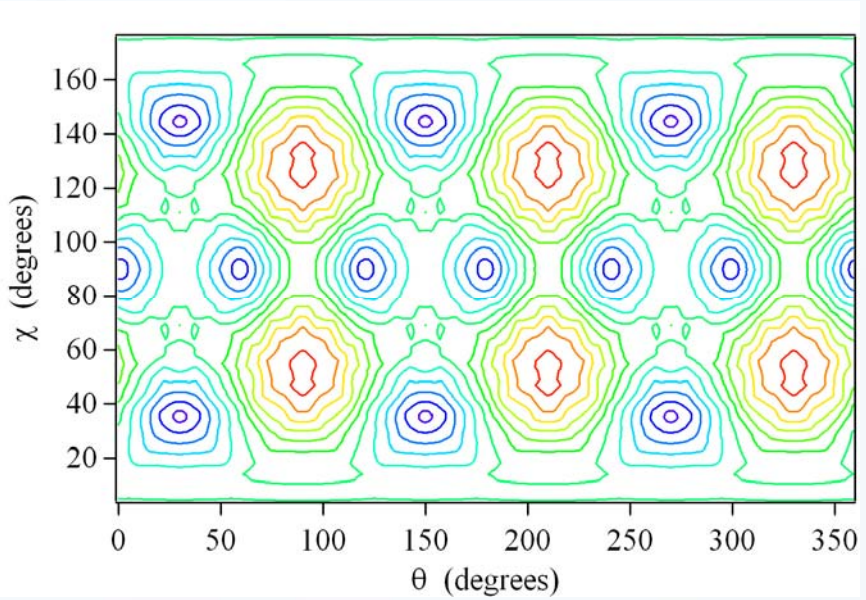




θ (in-plane)

χ (out-of plane)

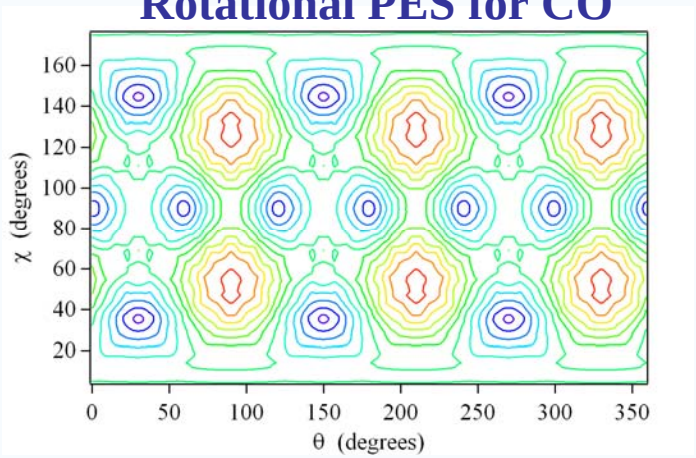
Rotational PES for CO in *h.c.p* H_2 lattice (Rigid)



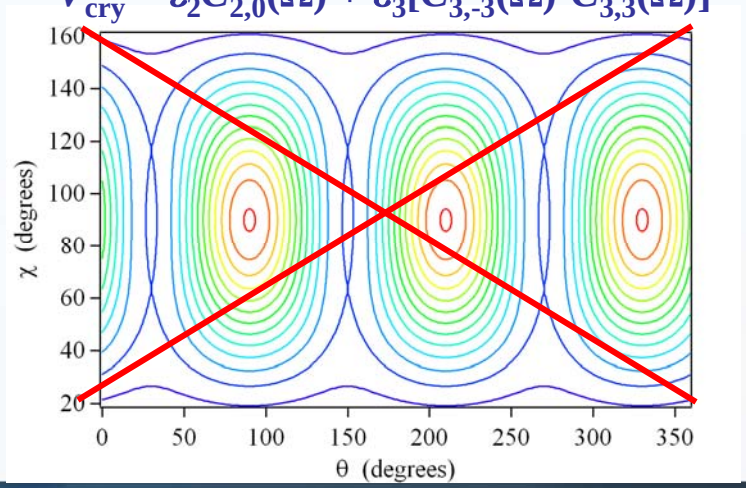
* SAPT / MC⁺BS, P. Jankowski and K. Szalwicz, *J. Chem. Phys.* 108, 3554 (1998).

Prediction of Crystal Field Parameters: Truncation

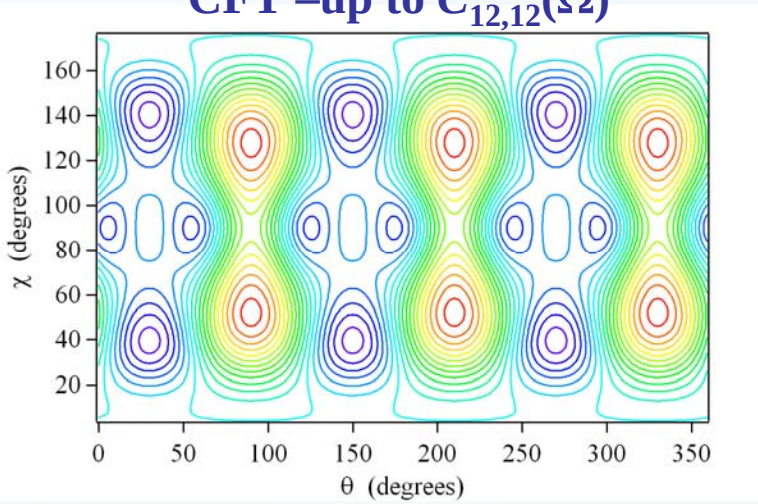
Rotational PES for CO



$V_{cry} = \varepsilon_2 C_{2,0}(\Omega) + \varepsilon_3[C_{3,-3}(\Omega) - C_{3,3}(\Omega)]$



CFT –up to $C_{12,12}(\Omega)$



(2.52)*

ε (cm^{-1})	Term	ε (cm^{-1})	Term
1.39	$C_{3,3}(\Omega)$	0.07	$C_{9,3}(\Omega)$
1.23	$C_{5,3}(\Omega)$	0.04	$C_{12,6}(\Omega)$
0.74	$C_{4,0}(\Omega)$	0.04	$C_{8,0}(\Omega)$
-0.57	$C_{6,6}(\Omega)$	0.03	$C_{12,12}(\Omega)$
-0.43	$C_{6,0}(\Omega)$	0.03	$C_{12,0}(\Omega)$
0.35	$C_{7,3}(\Omega)$	-0.03	$C_{11,3}(\Omega)$
0.13	$C_{8,6}(\Omega)$	-0.03	$C_{2,0}(\Omega)$

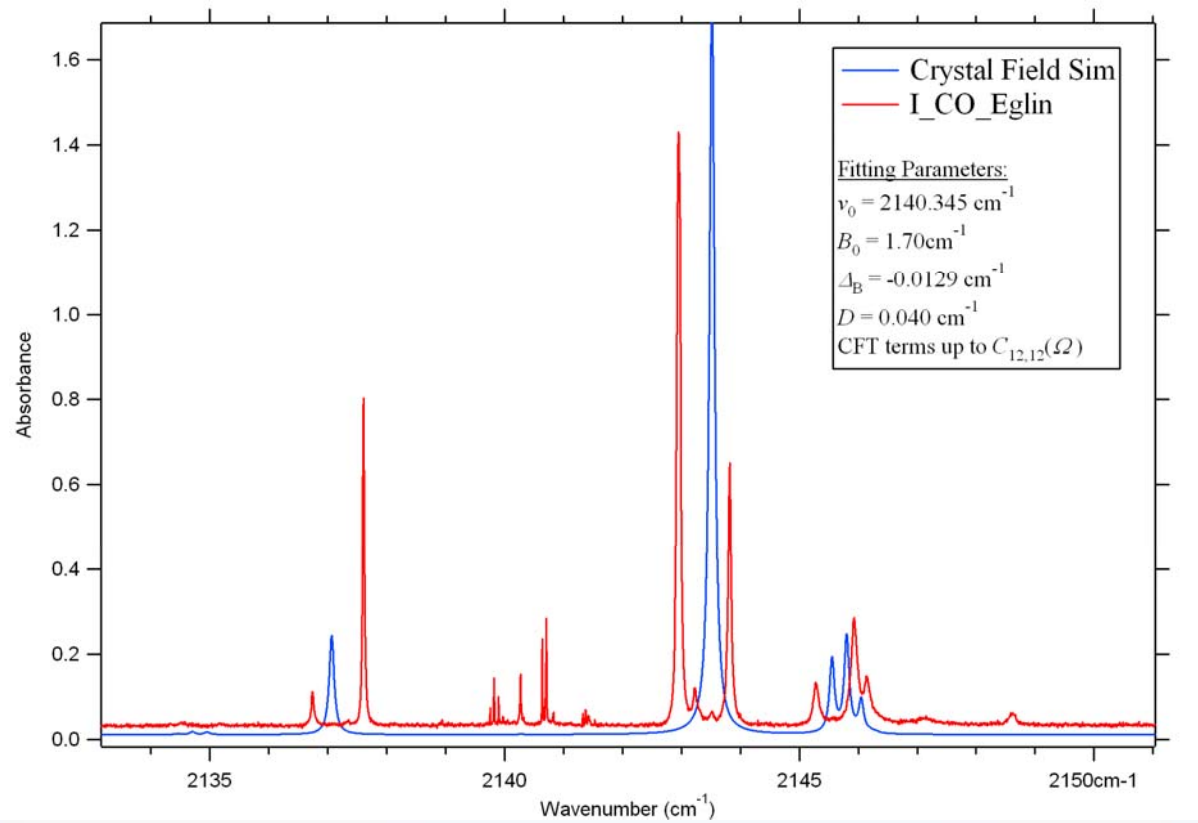
(1.03)*

* Experimentally fitted values.

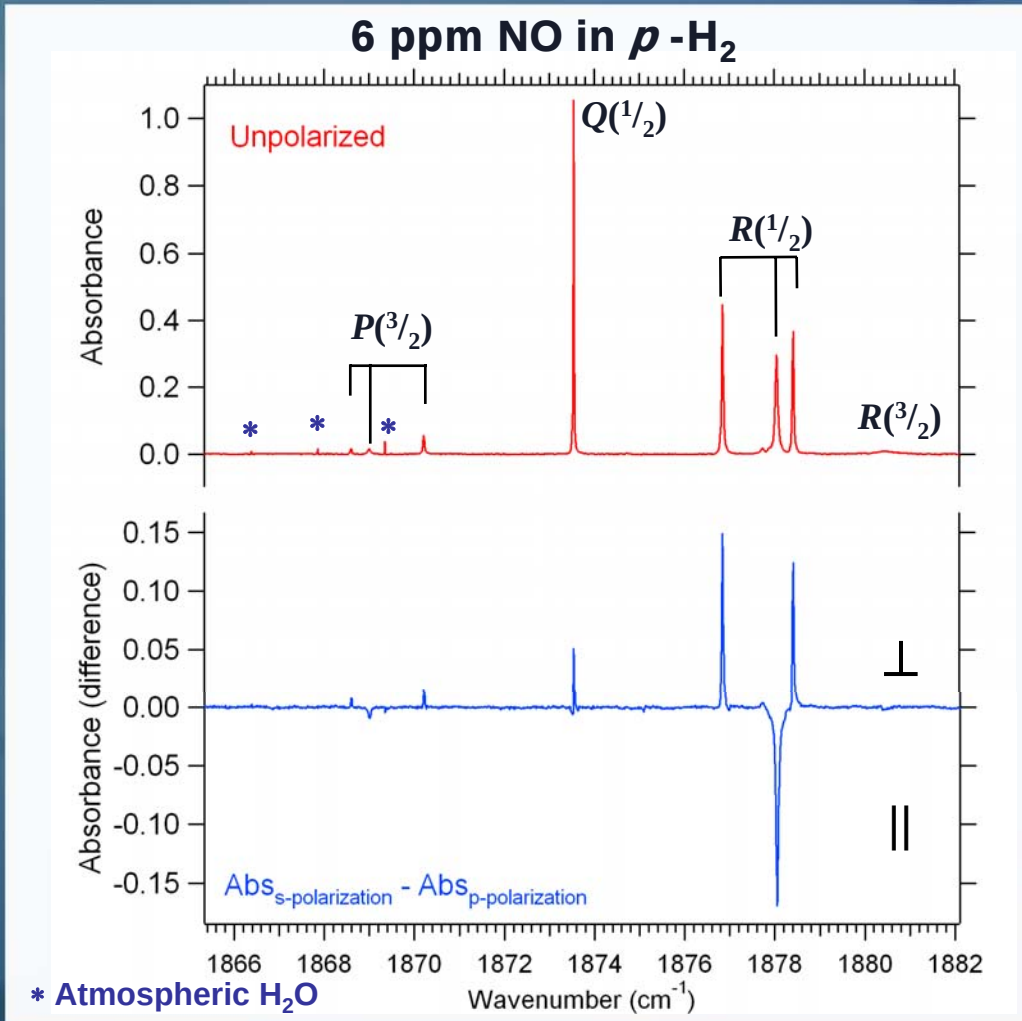
Estimation of Crystal Field Parameters: Simulated Spectrum for CO

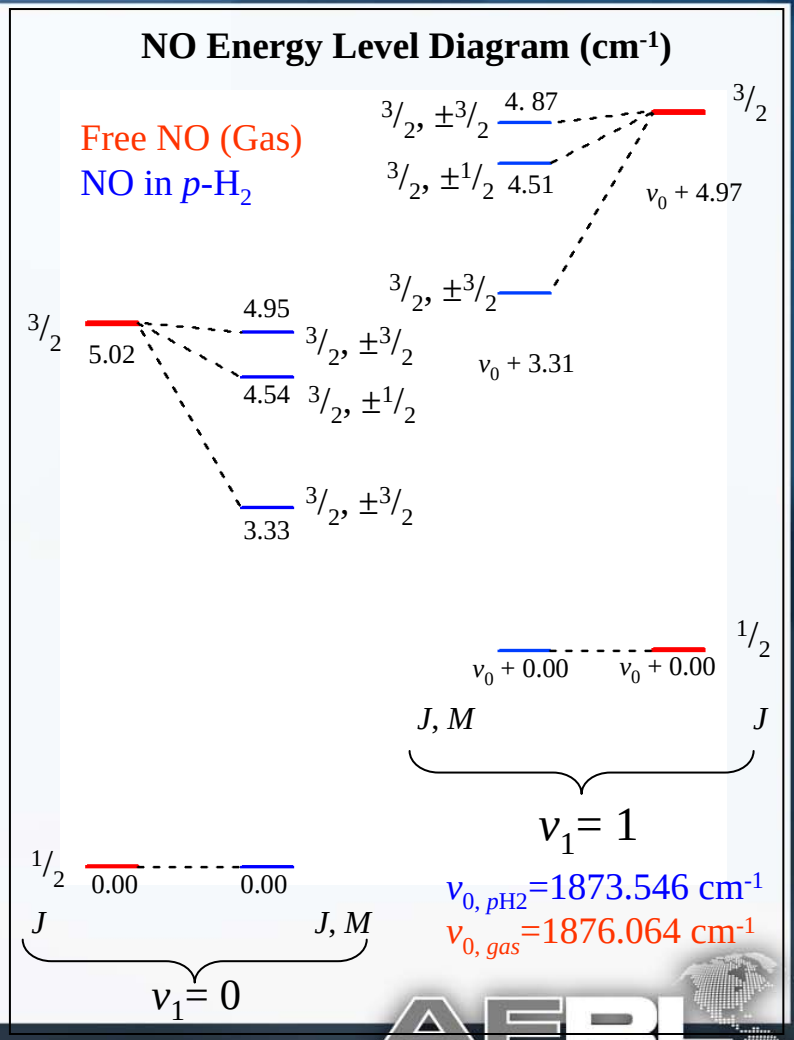
- Underestimates crystal field splittings.
- *S*(0) transition too weak.

- Mixing underestimated
- First order perturbation insufficient?

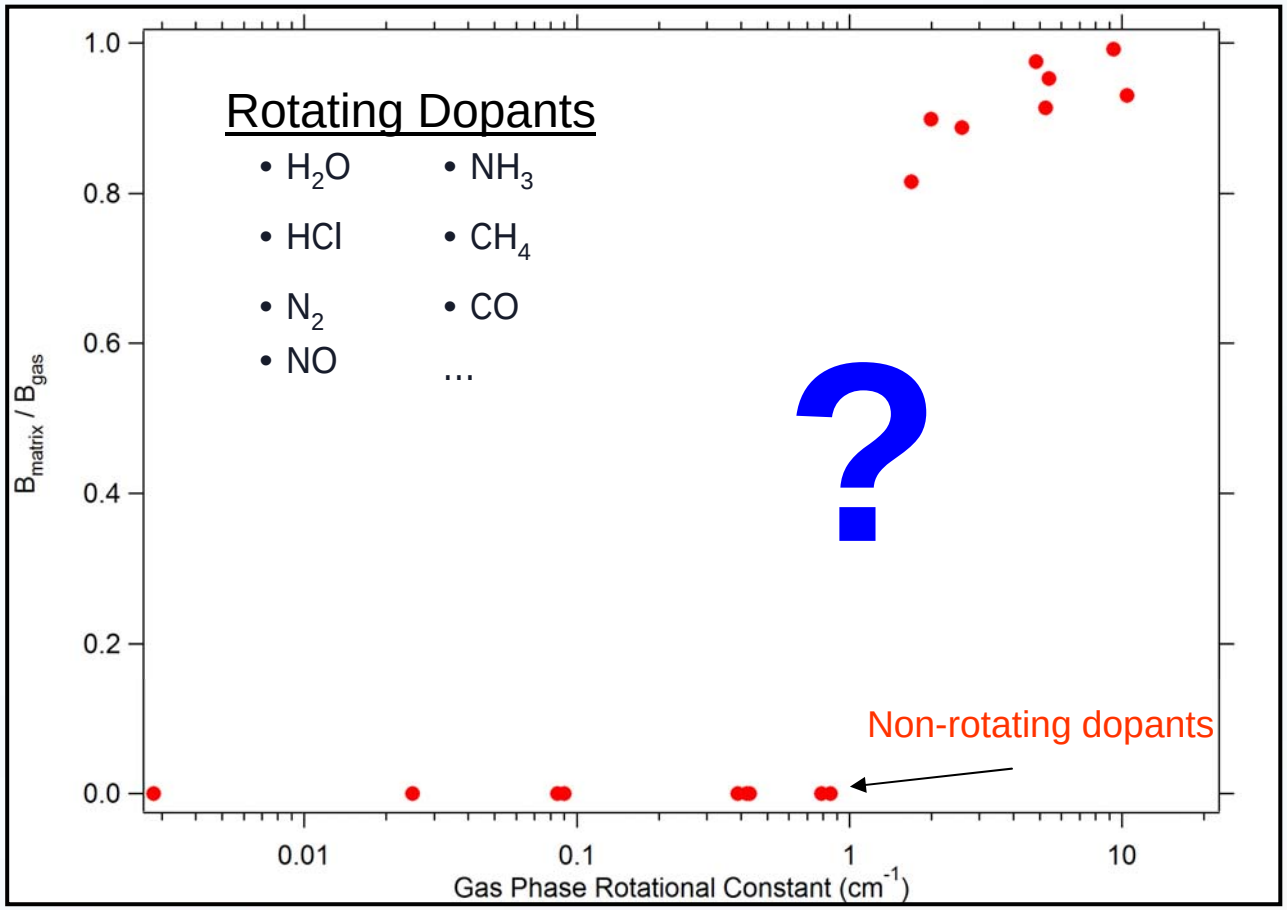


NO in Solid Parahydrogen



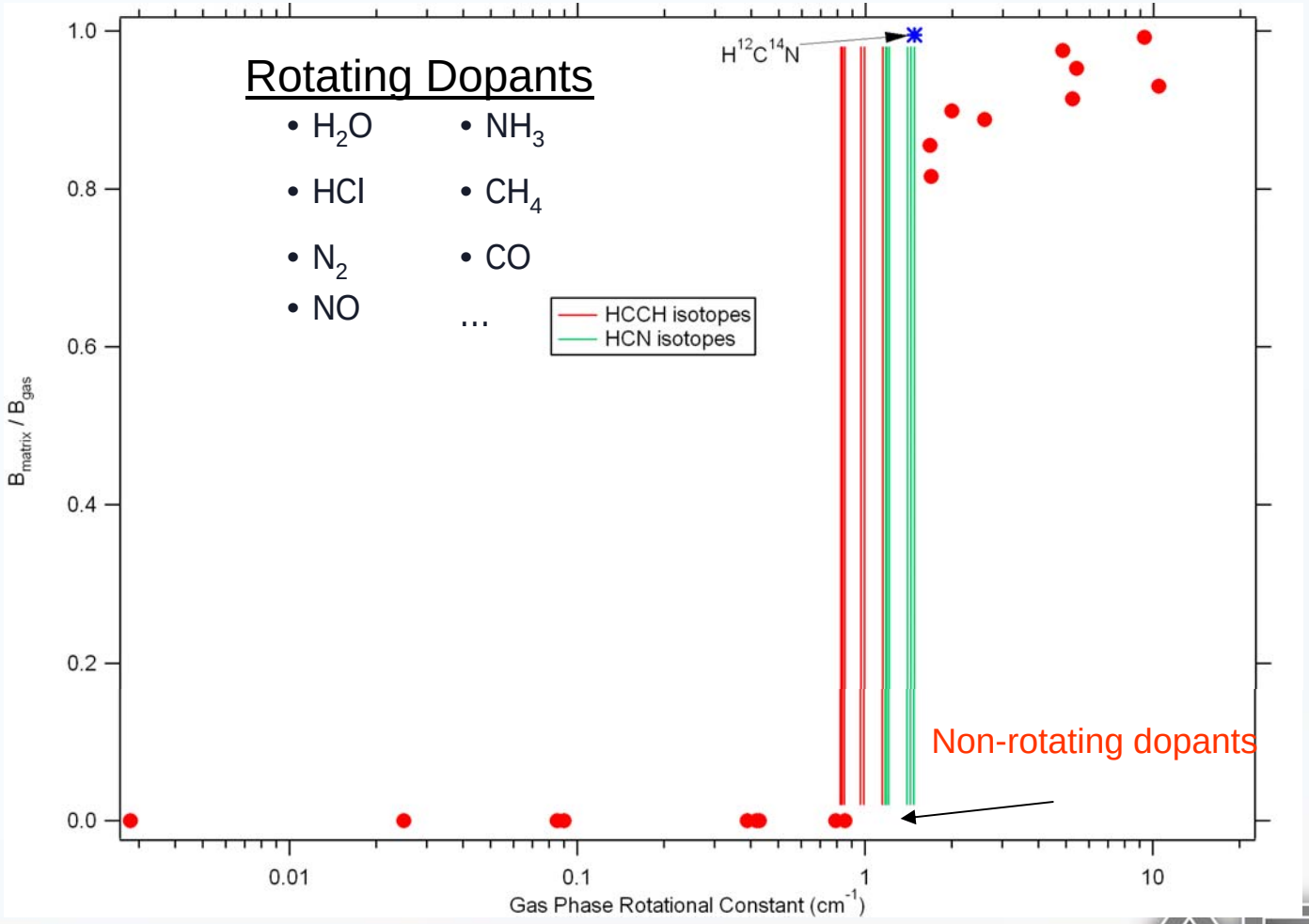


Rotors Within Parahydrogen

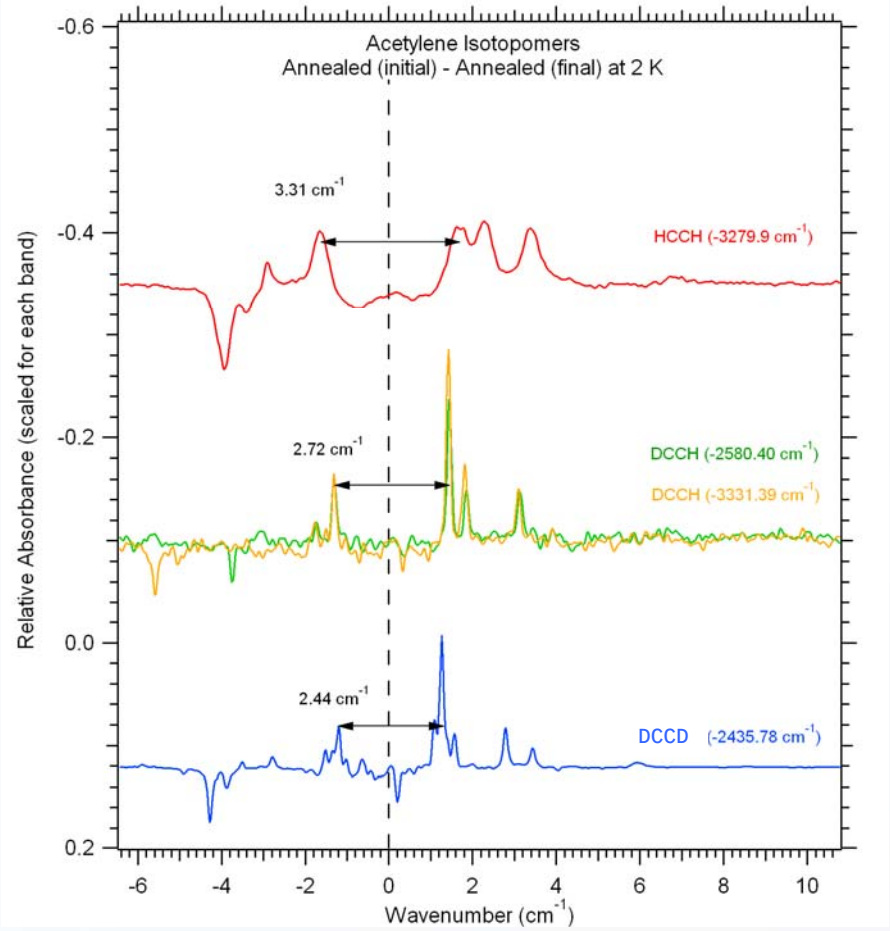


Data from the groups of M. E. Fajardo, Y.-P. Lee, and T. Momose (1995-2006).

Rotors Within Parahydrogen



Preliminary C_2H_2 in parahydrogen



$E_{R(0)} - E_{P(1)}$ $(4B)$

	Gas		pH_2	
	Wavenumer	Relative	Wavenumber	Relative
HCCH	4.71 cm^{-1}	**1.00**	3.35 cm^{-1}	**1**
DCCH	3.97 cm^{-1}	**0.84**	2.74 cm^{-1}	**0.82**
DCCD	3.39 cm^{-1}	**0.72**	2.47 cm^{-1}	**0.74**

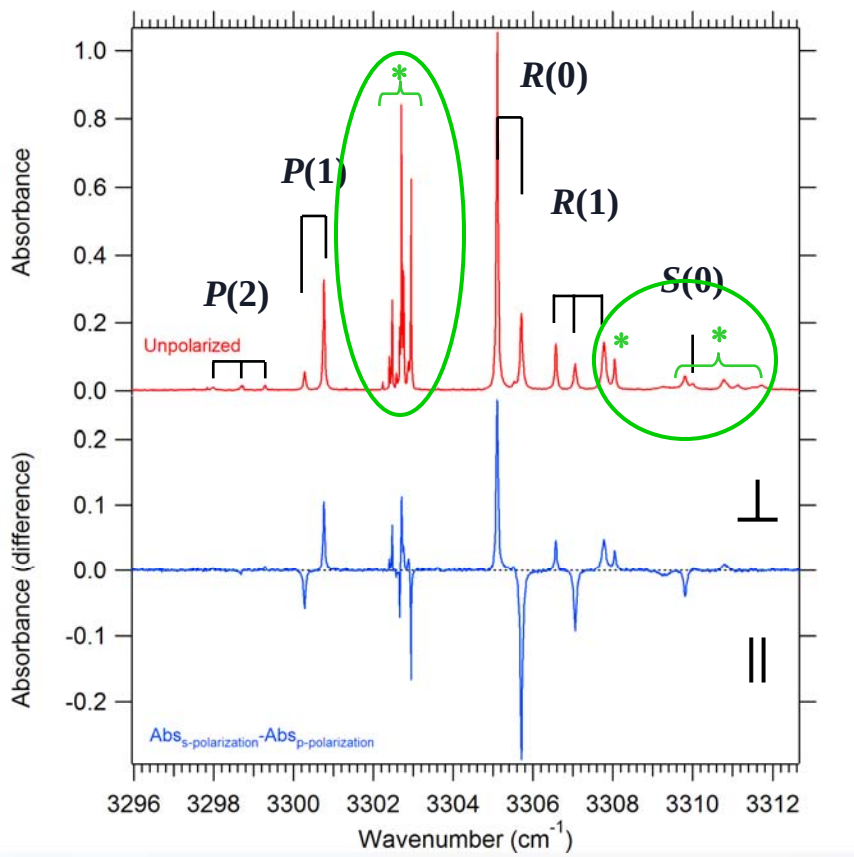
- Acetylene IR spectrum 'ages'... timescale of 30 minutes. Aging appears to be acetylene-acetylene clustering.
- "Rotational spectrum" disappears fairly quickly (but not with annealing!)

Y.P. Lee and collaborators *Chem. Phys. Lett.* 435 247-251 (2007) – no rotation at 'high' [o-H_2]

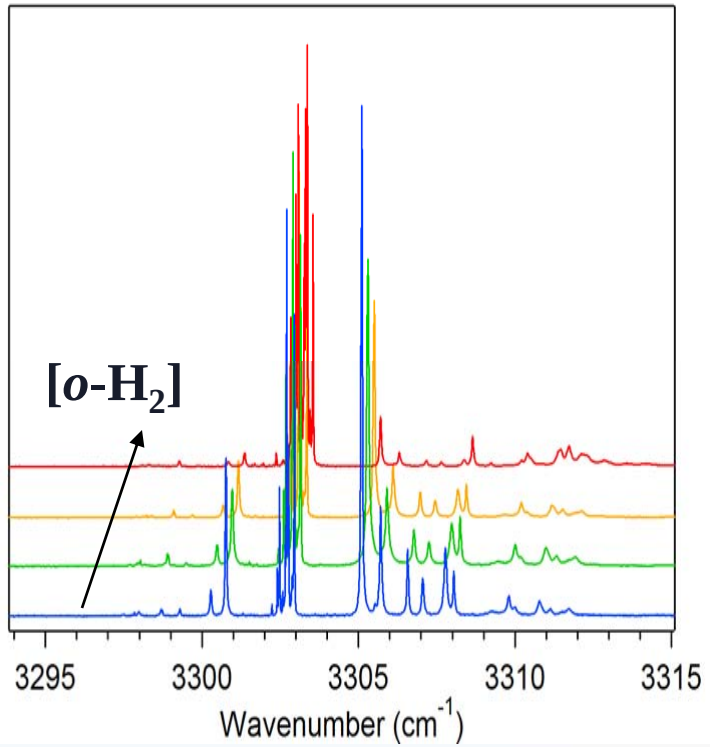
Dopant Cluster Formation in Solid Parahydrogen

o-H_2 – HCN Clustering

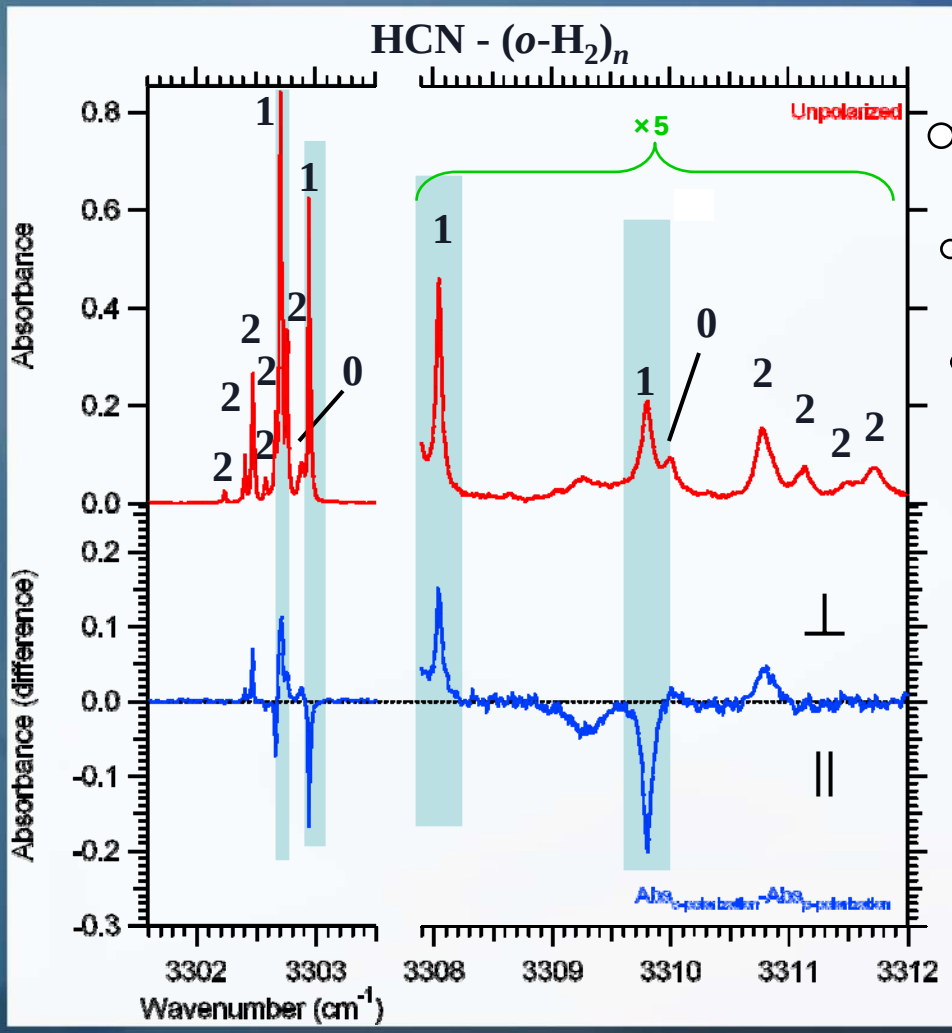
8 ppm HCN in *p*-H_2



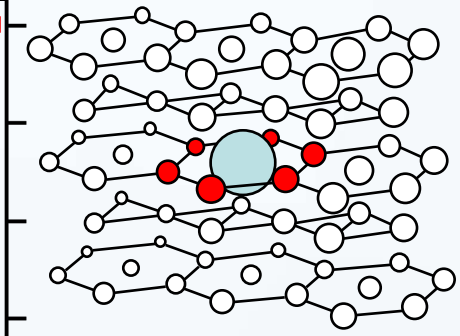
Orthohydrogen Dependence



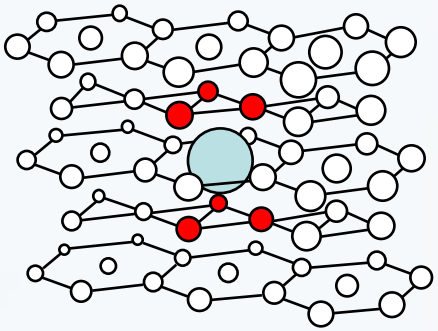
o-H_2 – HCN Clustering



In-plane



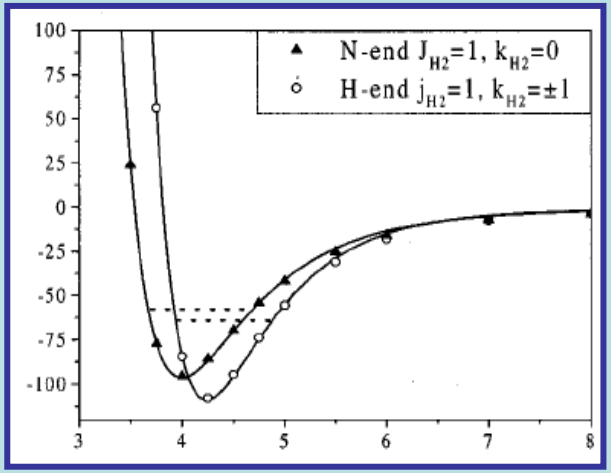
Out-of-plane



Two binding sites predicted *

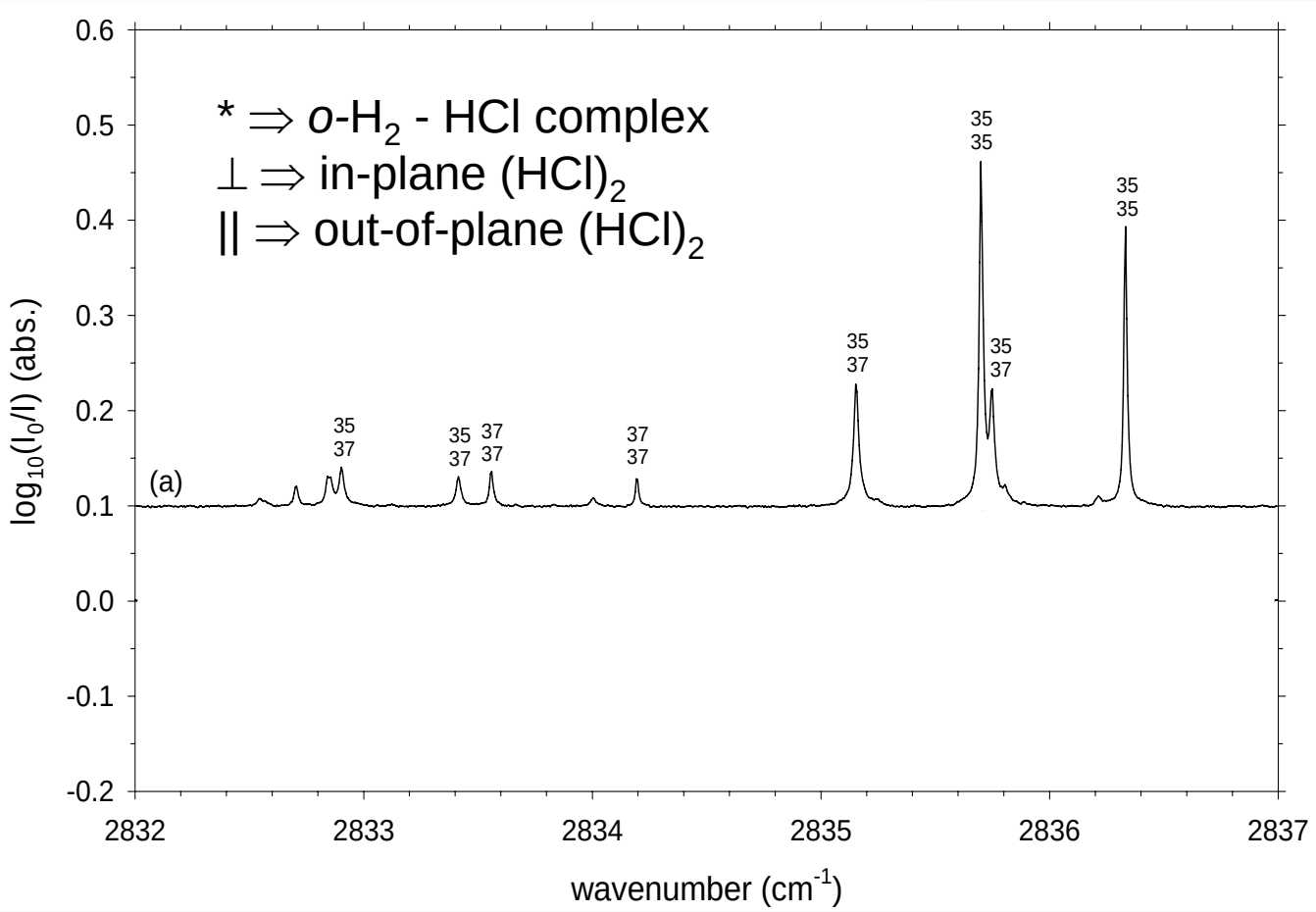
HCN-*o*H_2

oH_2 - HCN



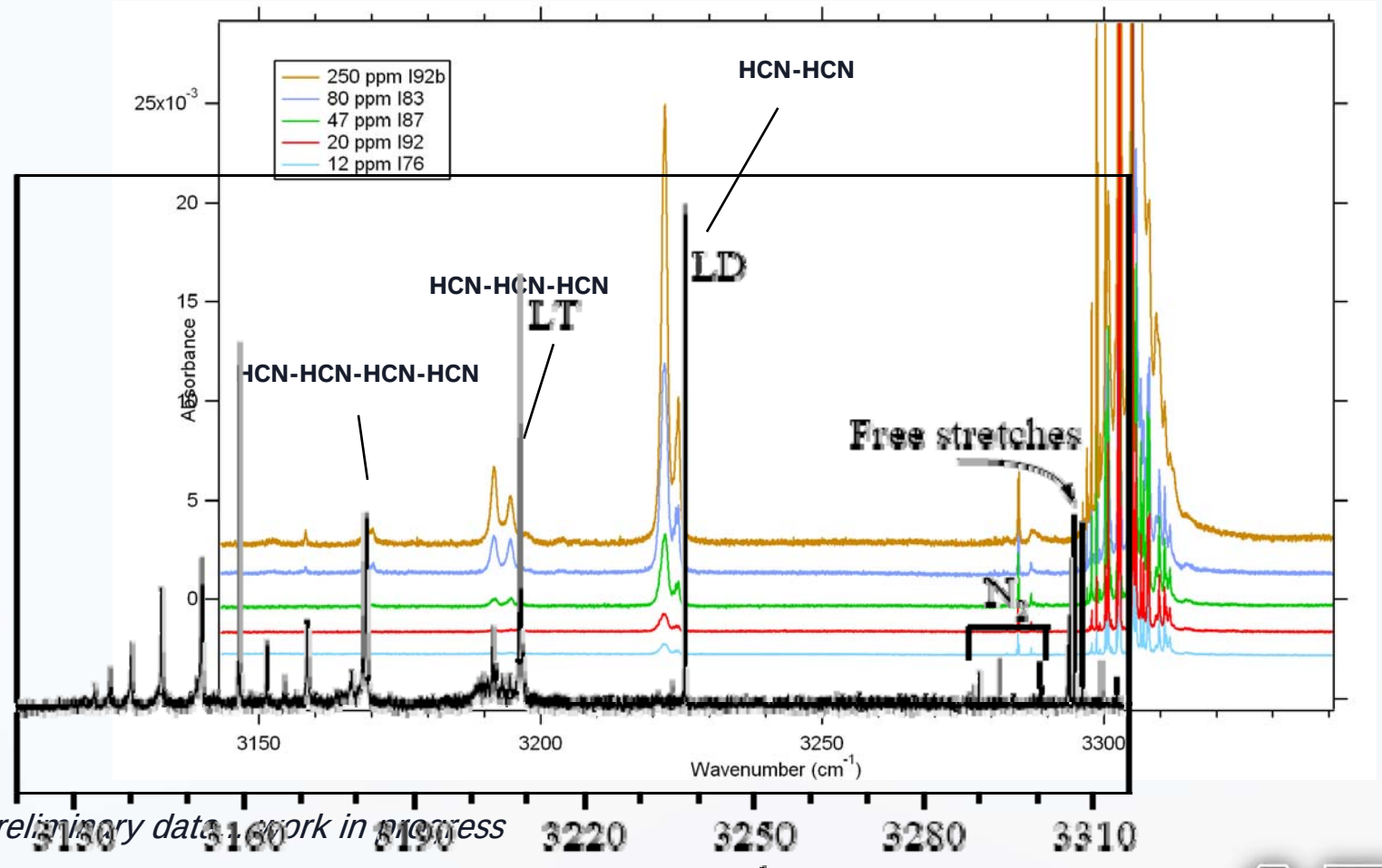
* *Moore, Ishiguro, and Miller, JCP 115, 5144 (2001)*

HCl dimer



See Mario Fajardo's Poster for more details

HCN Clustering in *p*-$H_{2(s)}$ – linear assembly in the solid state?



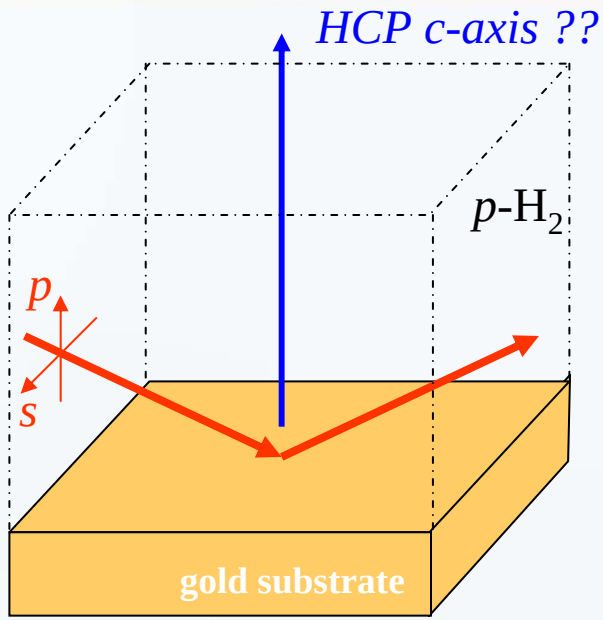
Preliminary data - work in progress

Crystallite Orientation and the Annealing Behavior of Doped Solid Parahydrogen

Orientation of Crystal Axis

- Lab frame versus crystal frame of reference.
- '*s*' – '*p*' polarization provides moment relative to surface normal.
- Spectral fine structure sensitive to the local crystallite orientation.

Correlation between crystal axis and surface normal?

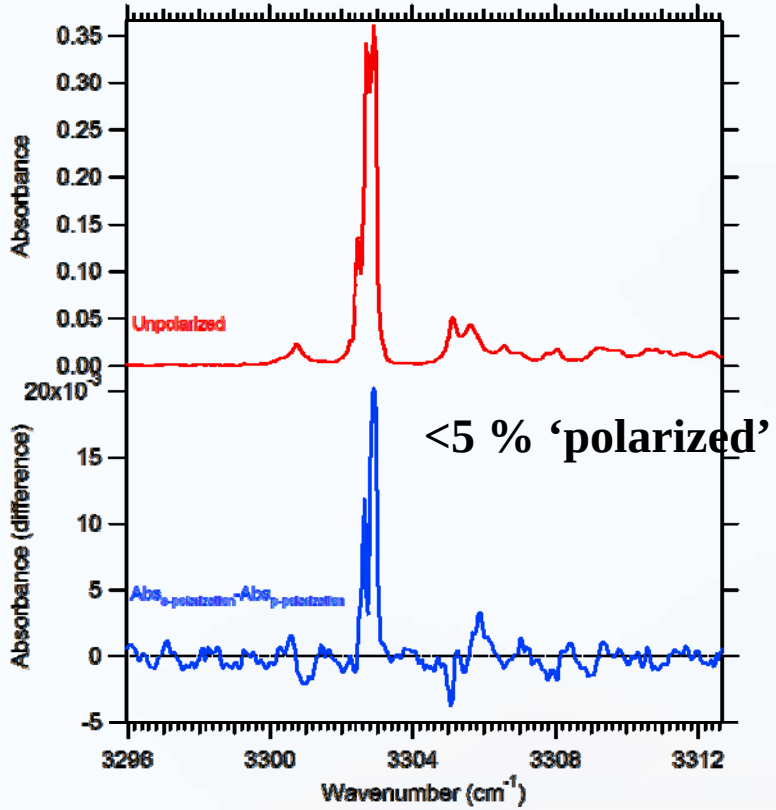


Polarization analysis provides:

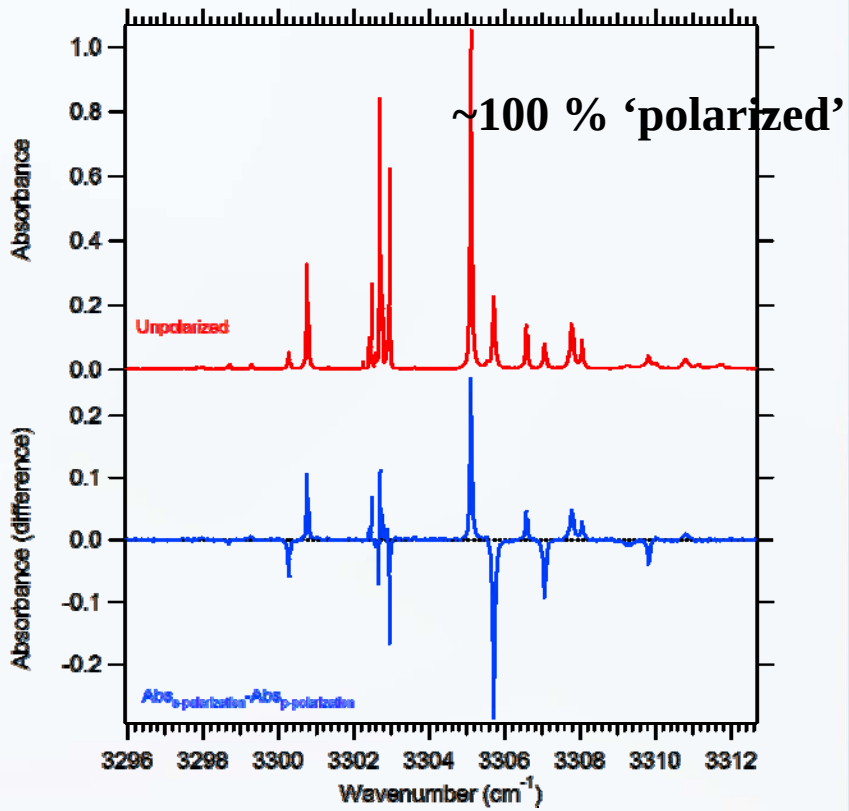
- **An assignment of the perpendicular and parallel components to the crystal field perturbed rotational structure (*i.e.* Δm)**
- $\mathbf{Abs_{s\text{-}pol} - Abs_{p\text{-}pol} = \frac{1}{2}\,\mu^2_{\perp} - \frac{1}{2}\,\mu^2_{\parallel}}$

As Deposited Versus Annealed

As-deposited, 8 ppm HCN in *p*-H_2 @ 2.3 K



Annealed, 8 ppm HCN in *p*-H_2 @ 2.3 K



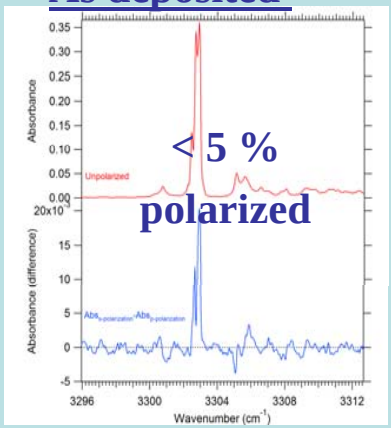
- Before annealing, less than 5% of the HCP features are oriented normal to the substrate.
- *After annealing*, ~90% of the HCP features are oriented normal to substrate!!

→ Upon deposition, HCP lattices randomly oriented, but upon annealing gain a macroscopic orientation to the laboratory frame.

Multiple samples – HCN, CO, NO

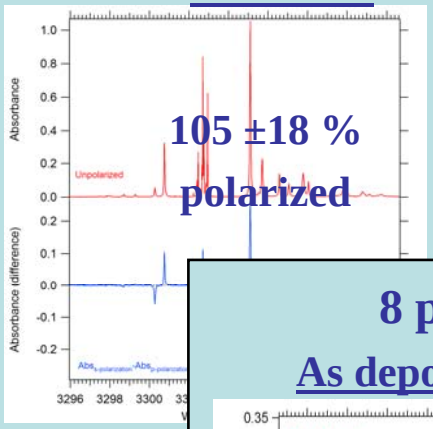
8 ppm HCN in parahydrogen

As deposited



< 5 % polarized

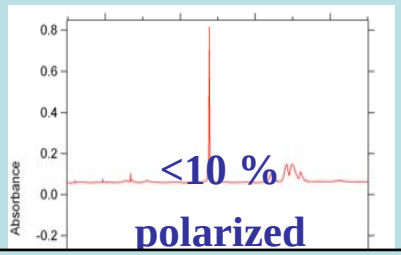
Annealed



105 ±18 % polarized

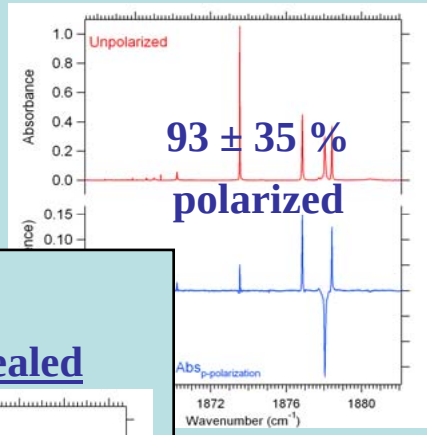
8 ppm NO in parahydrogen

As deposited



<10 % polarized

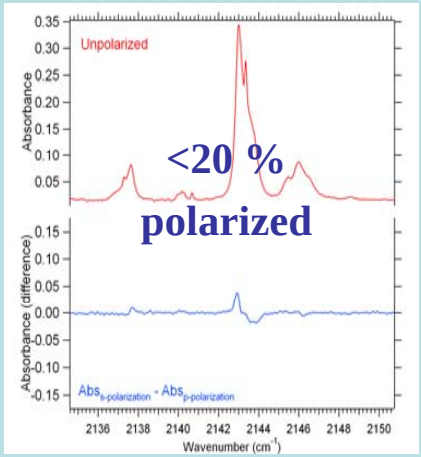
Annealed



93 ± 35 % polarized

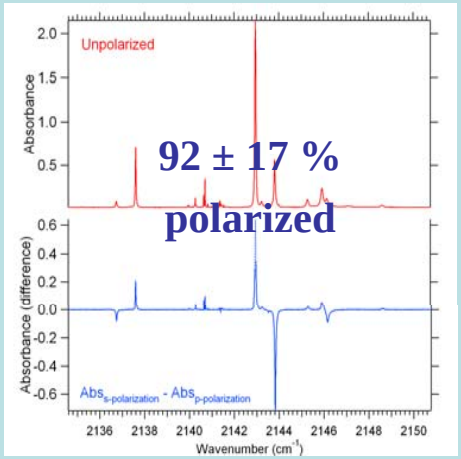
8 ppm CO in parahydrogen

As deposited



<20 % polarized

Annealed



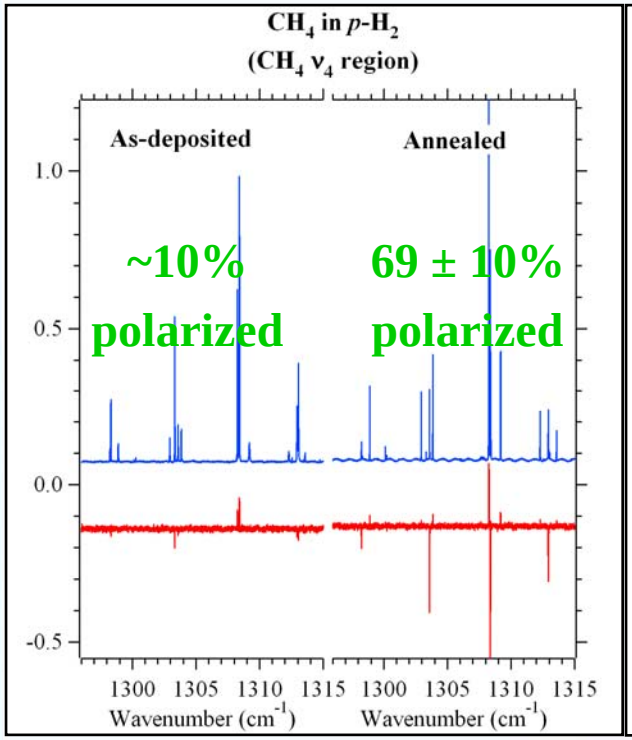
92 ± 17 % polarized

- **All exhibit virtually no alignment in as deposited samples**

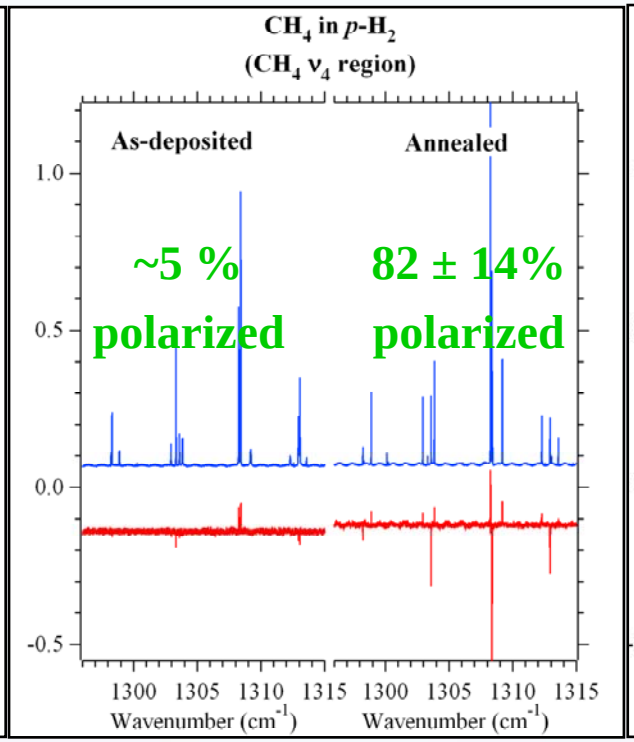
- **All exhibit more than 90% alignment of crystal axis after annealing.**

CH_4 in parahydrogen

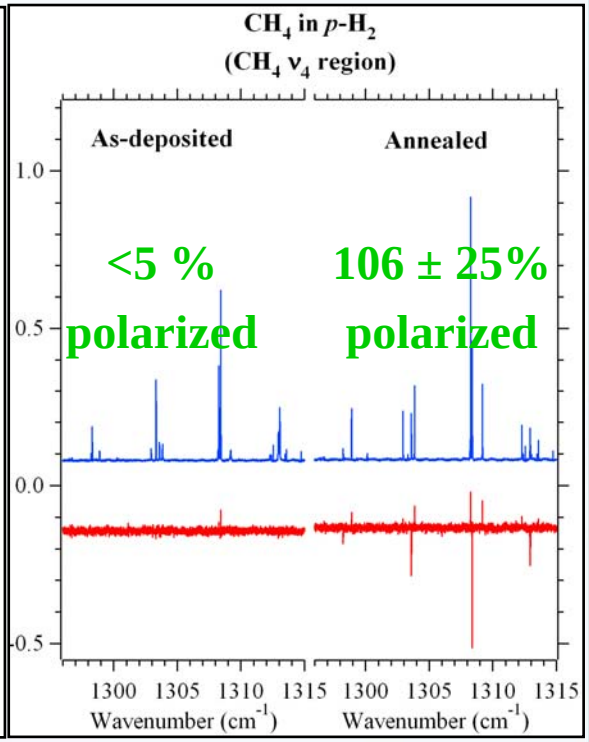
Sample 1



Sample 2



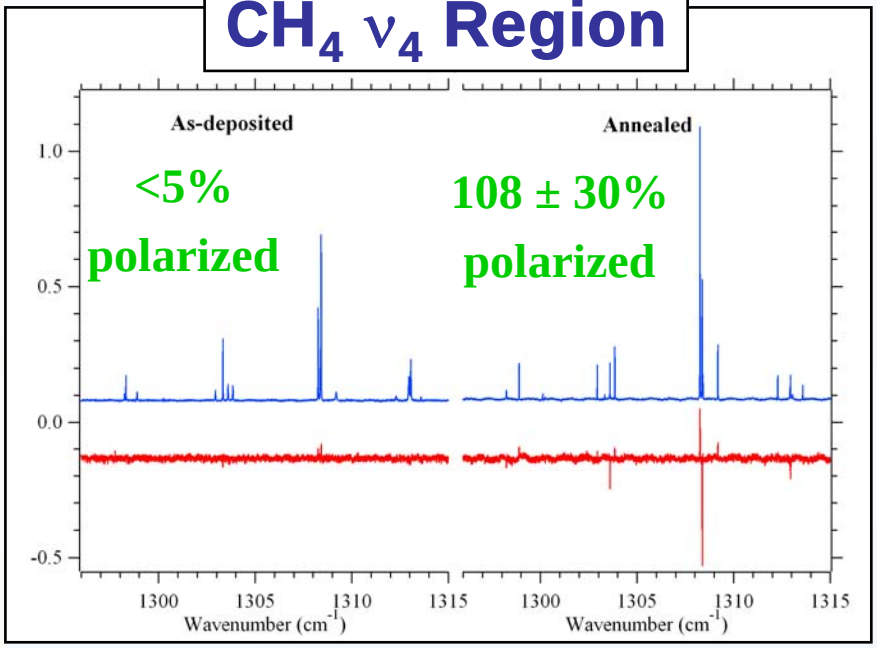
Sample 3



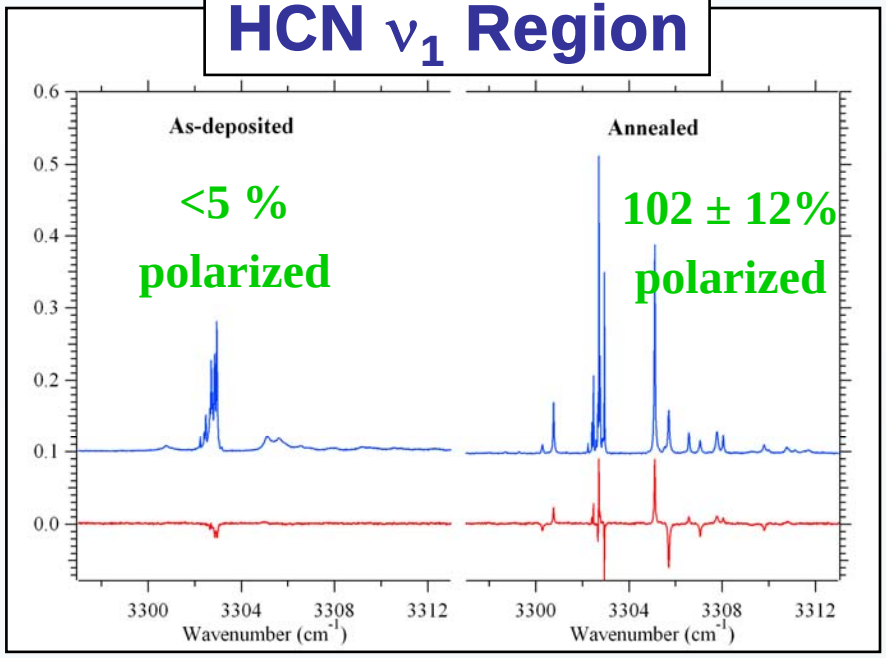
- Essentially no orientation in as deposited.
- Degree of polarization in annealed samples fluctuates for CH_4 from sample to sample.
- Dopant helps establish macroscopic orientation?

Mixed CH_4 and HCN (3.5 ppm / 3.8 ppm)

CH_4 ν_4 Region



HCN ν_1 Region



- % orientation agrees in mixed samples
- HCN more influential than CH_4?

Conclusions

- Solid parahydrogen produced by Rapid Vapor Deposition is amenable to Polarization Spectroscopy:
  - Facilitates the assignment of the crystal field fine structure in the spectra of rotating dopants.
  - Sheds light on cluster formation in doped parahydrogen samples.
  - Provides new insight into the annealing behavior of the solid parahydrogen produced by RVD.

Electron and Positron irradiation of solid hydrogen presently underway

Acknowledgements:

Takamasa Momose, U. British Colombia (Crystal Field Theory)

David Anderson, U. Wyoming (NO and $(HCl)_2$ work)

David Moore, Lehigh U. (H_2-HCN *ab initio* potential)

Basic Research in Military

… It's alive and active

- Great job opportunities for recent grads
- Good, fundamental research efforts underway
- Opportunities for academia to help! The real challenge is in "selling" your work and providing a valid, realistic path towards an application... (more than just lip service is required)

A few final thoughts…

" Scientists do a great job with the details of the science. Scientists must learn the art of the sound bite!"

- Bill Nye (the science guy)

Interview with C&E News, 2006

"In this Worldwide economy our ability to create wealth is not/no longer bounded by physical limits/natural resources but by our ability to come up with KEY "new ideas"/Inventions. The More Education, the more Ideas and the More WEALTH, Education is THE KEY *"*

- Dennis Bushnell (2002)

Chief Scientist, NASA Langley

"The best way to predict the future is to invent it."

- Alan Kay

Computer Scientist, 1991)

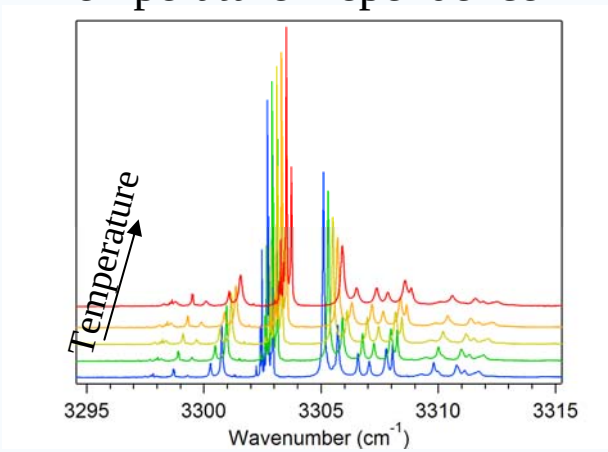
QUESTIONS?

AFRL
THE AIR FORCE RESEARCH LABORATORY
LEAD I DISCOVER I DEVELOP I DELIVER

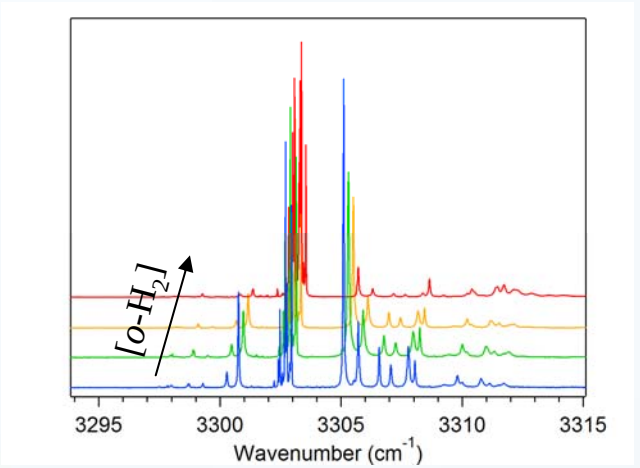
Back-up Slides

Spectral Assignments Tools

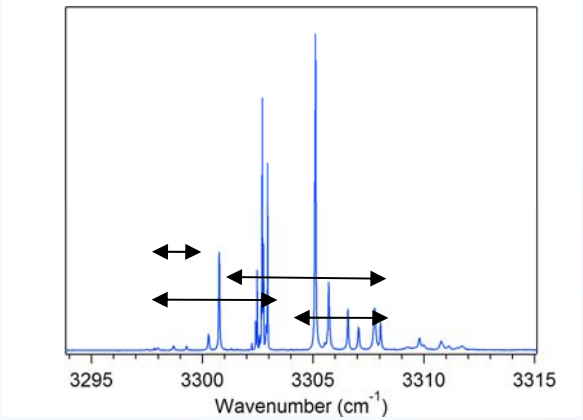
Temperature Dependence



Orthohydrogen Dependence



Combination Differences



Spectrum was interpreted by its:

- **Temperature dependence**
- **Orthohydrogen concentration dependence**
- **Transition frequency combination differences**
- **Polarization dependence!**

NO in solid parahydrogen